

NOVA: GENERATIVE LANGUAGE MODELS FOR ASSEMBLY CODE WITH HIERARCHICAL ATTENTION AND CONTRASTIVE LEARNING

Nan Jiang

Purdue University

jiang719@purdue.edu

Chengxiao Wang

University of Illinois Urbana-Champaign

cw124@illinois.edu

Kevin Liu

Lynbrook High School

kevin.bx.liu@gmail.com

Xiangzhe Xu

Purdue University

xu1415@purdue.edu

Lin Tan

Purdue University

lintan@purdue.edu

Xiangyu Zhang

Purdue University

xyzhang@cs.purdue.edu

Petr Babkin

J.P. Morgan AI Research

petr.babkin@jpmorgan.com

ABSTRACT

Binary code analysis is the foundation of crucial tasks in the security domain; thus building effective binary analysis techniques is more important than ever. Large language models (LLMs) although have brought impressive improvement to source code tasks, do not directly generalize to assembly code due to the unique challenges of assembly: (1) the low information density of assembly and (2) the diverse optimizations in assembly code. To overcome these challenges, this work proposes a *hierarchical attention* mechanism that builds attention summaries to capture the semantics more effectively, and designs *contrastive learning objectives* to train LLMs to learn assembly optimization. Equipped with these techniques, this work develops *Nova*, a generative LLM for assembly code. Nova outperforms existing techniques on binary code decompilation by up to 14.84 – 21.58% (absolute percentage point improvement) higher Pass@1 and Pass@10, and outperforms the latest binary code similarity detection techniques by up to 6.17% Recall@1, showing promising abilities on both assembly generation and understanding tasks.

1 INTRODUCTION

Binary code plays an irreplaceable role in the security domain, being the foundation of crucial tasks including vulnerability detection (Güler et al., 2019; Duan et al., 2020; Chen et al., 2022b), malware detection (Spensky et al., 2016; Aonzo et al., 2023; Xu et al., 2014), binary recovery (Su et al., 2024; Zhang et al., 2021; Chen et al., 2022c), and legacy software maintenance (Carbone et al., 2009; Carlini et al., 2015; Martin et al., 2010). For example, when performing tasks such as identifying attacks and malware, security analysts often only have access to assembly, i.e., the human-readable representation of binary code, which is extremely difficult to understand (Su et al., 2024; Zhang et al., 2021; Chen et al., 2022c). Thus, combined with the increasing sophistication of cybercrime that poses significant threats worldwide (e.g., cybercrime is predicted to cost the world \$10.5 trillion annually by 2025 (Sausalito, 2020)), effective binary analysis techniques are in high demand.

<pre>#include <stdio.h> #include <math.h> int compare(int *x, int *y) { if (*int*x < *(int*)y) return -1; if (*int*x > *(int*)y) return 1; return 0; }</pre>	<pre>0: endbr64 4: push %rbp 5: mov %rsp,%rbp 8: mov %rdi,-0x8(%rbp) c: mov %rsi,-0x10(%rbp) 10: mov -0x8(%rbp),%rax 14: mov (%rax),%edx 16: mov -0x10(%rbp),%rax 1a: mov (%rax),%eax 1c: cmp %eax,%edx</pre>	<pre>0: endbr64 4: mov (%rdi),%ecx 6: mov (%rsi),%edx 8: mov \$0xffffffff,%eax d: cmp %edx,%ecx f: jl 17 11: setg %al 14: movzb %al,%eax 17: retq</pre>
(a) Source Code Function	(b) Assembly (O0-Optimized)	(c) Assembly (O1-Optimized)

Figure 1: Example that shows the semantics and diverse optimizations of assembly code.

Large language models pre-trained on source code have brought improvement in various software development domains (Chen et al., 2022a; Liu et al., 2023a; Chen et al., 2023; Le et al., 2022; Jiang et al., 2023; Xia et al., 2023). However, these LLMs are not designed for or trained with assembly corpus, not achieving their full potential on binary code analysis tasks such as binary code similarity (Wang et al., 2022; Xu et al., 2023a), malware detection (Su et al., 2024), and binary code decompilation (Tan et al., 2024; Armengol-Estabé et al., 2024; Hosseini & Dolan-Gavitt, 2022).

Existing work applying LLMs on assembly code mainly piggybacks on encoder-style LLMs (Wang et al., 2022; Su et al., 2024; Xu et al., 2023a), unable to benefit from the more extensive pre-training, updated architectures, scaling of state-of-the-art generative LLMs. Other work using generative LLMs for decompilation shows a low unit test passing rate of the decompiled programs (Tan et al., 2024; Armengol-Estabé et al., 2024).

The challenges of leveraging generative LLMs for assembly code are twofold. First, compared to source code, assembly code has a *lower information density*. A short source-code sequence maps to an assembly-code sequence that is often several times longer. Thus, assembly semantics span across a *long sequence of tokens*. Figure 1 (a) shows an example of a source code function that compares two integers, while Figure 1 (b) shows its corresponding assembly code optimized with `00` flag. In the `00`-optimized assembly code, the five instructions from `10: mov -0x8(%rbp),%rax` to `1c: cmp %eax,%edx` perform the checking whether the value of `x` is smaller than the value of `y` (correspond to `if (*int*)x < (*int*)y` in the source code). A single assembly instruction alone represents little meaningful semantics in the source code. It is the combinations of *many instructions* and the *dependencies* between them represent the semantics. Such combinations of instructions are long, which is hard for LLMs to learn.

Second, assembly code is diverse due to compiler optimization. The assembly code of the same source code function looks dramatically different with different compiler optimization. Figure 1 (c) shows the assembly of the same function compiled with `01` and `00` flags, which consists of a significantly different set of instructions. Such syntax diversity is hard for LLMs to learn, preventing LLMs from obtaining consistently good performances on differently optimized assembly code.

In this work, we develop Nova, a generative foundation LLM pre-trained for assembly code with two key novelties. First, to address the low-information-density and long-sequence challenge, we design a hierarchical self-attention, which contains three categories of attention at different levels of granularity: intra-instruction attention, preceding-instruction attention, and inter-instruction attention. The key insight is to build *attention summaries*, i.e., we create per-statement attention *labels*, which act as the summary of a statement. We then use preceding-instruction attention to capture semantics between a token and its preceding instruction label and use inter-instruction attention for long dependencies. Besides, we design *functionality contrastive learning* and *optimization contrastive learning* objectives to train Nova to learn the semantics behind the diverse syntax of assembly.

This work makes the following contributions:

- We propose a novel hierarchical attention mechanism that captures the assembly’s low-density semantics at three granularity levels.
- We design contrastive learning objectives to train LLMs to learn assembly with diverse optimizations and encode assembly more efficiently.
- We develop Nova, a generative foundation LLM with hierarchical attention and contrastive learning for assembly. Nova outperforms state-of-the-art on binary decompilation by up to 14.84 – 21.58% higher Pass@1 and Pass@10, and on binary similarity detection by up to 6.17% Recall@1.
- Availability: we release Nova models at <https://huggingface.co/lt-asset/nova-1.3b> and <https://huggingface.co/lt-asset/nova-6.7b>

2 RELATED WORK

2.1 BINARY MODELS

Machine learning models are widely used in binary program analysis tasks. However, these models are typically designed for specific tasks such as binary code similarity detection (Pei et al., 2020; Xu et al., 2023a; Wang et al., 2022; Xu et al., 2017; Ding et al., 2019), variable name prediction (Chen et al., 2022c; Xu et al., 2023b; Zhang et al., 2021; He et al., 2018; Lacomis et al., 2020), binary

code type inference (Pei et al., 2021), and so on (Chen et al., 2022d; Liu et al., 2023b; Hosseini & Dolan-Gavitt, 2022).

Recent techniques have started to pre-train foundation LLMs for binaries. CodeArt (Su et al., 2024) pre-trains encoder-style LLMs with a regularized attention design to better encode assembly code semantics. SLaDe (Armengol-Estabé et al., 2024) trains BART (Lewis et al., 2019) models on assembly. Meta LLMCompiler (Cummins et al., 2024) train CodeLlama models on LLVM IR to optimize binary code. LLM4Decompile (Tan et al., 2024) trains DeepSeekCoder with assembly for binary code decompilation. However, CodeArt does not generalize to generation tasks due to its encoder architecture. LLMCompiler trained on LLVM IR cannot be effectively transferred to assembly code. SLaDe and LLM4Decompile are limited in performance due to a lack of special designs for assembly. In contrast, Nova proposes hierarchical attention and contrastive learning objectives, outperforming existing techniques on both understanding (binary code similarity detection) and generation (binary code decompilation) tasks.

2.2 LARGE SOURCE-CODE MODELS

LLMs demonstrate promising results on many code-related tasks, such as code generation (Chen et al., 2022a; Liu et al., 2023a; Chen et al., 2023; Le et al., 2022; Yue et al., 2021; Chen et al., 2021; Nijkamp et al., 2022; Fried et al., 2023; Rozière et al., 2023; Guo et al., 2024; Lozhkov et al., 2024; Hui et al., 2024), bug fixing (Jiang et al., 2023; Xia et al., 2023) and vulnerability fixing (Wu et al., 2023; Steenhoek et al., 2023; He & Vechev, 2023). The advances in using LLMs are attributed to the knowledge learned from massive source code and natural language text in their training datasets (Touvron et al., 2023; OpenAI, 2023). Nova is designed and trained for assembly, which has unique challenges such as low information density and diverse optimization.

2.3 ATTENTION MECHANISM

Standard self-attention is widely used in transformer architecture (Vaswani et al., 2017) to capture soft dependencies between tokens in the input. Many special attention mechanisms have been designed for better learning in various scenarios (Yang et al., 2016; Huang et al., 2024). LongCoder (Guo et al., 2023) combines window attention and global attention (attention sink (Xiao et al., 2024)) to handle long input of source code. We have shown that LongCoder’s window attention is less effective than Nova’s on assembly code. CAST (Shi et al., 2021) is a new neural architecture that splits the abstract syntax tree (AST) of source code into subtrees, encodes the subtrees, and aggregates to the final encoding. PA-former (Chai & Li, 2024) is a new neural architecture that constructs source code as pyramid input based on their AST structure and contains a pyramid attention mechanism to calculate the features in a hierarchical way. HierarchyNet (Nguyen et al., 2023) is a neural architecture that considers source code AST, data flow, and control flow graphs. Similarly, it cannot be applied to assembly code. Different from CAST, PA-former, and HierarchyNet, Nova’s attention design is for assembly code, is more lightweight and can be plugged into any pre-trained generative LLM.

3 APPROACH

Figure 2 presents the overall approach of Nova. We build Nova on top of foundation models for source code (Guo et al., 2024) to utilize their source code and natural language generation ability. We first collect large assembly corpora (Section 3.1). Section 3.2 describes Nova’s hierarchical attention design. With the collected assembly corpora, we then pretrain Nova with language modeling and contrastive learning objectives (Section 3.3). Then, we fine-tune Nova on two important downstream tasks, binary code decompilation, and binary code similarity detection (Sections 3.4 and 3.5), to prove Nova’s effectiveness and benefits to the binary research domain.

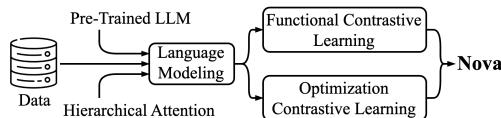


Figure 2: Overview of developing Nova

Table 1: Statistics (number of C and X86-64 assembly functions) of the pre-training datasets.

Origin	C Functions	O0	O1	O2	O3	Total
AnghaBench	757.1K	743.1K	726.4K	718.7K	717.8K	3.7M
The-Stack	138.8K	125.1K	119.7K	116.9K	108.8K	609.3K

3.1 DATA COLLECTION

In this paper, we focus on X86-64 assembly functions for C programs. Yet, Nova’s approach is generalizable to other assembly languages such as ARM assembly.

We derive our X86-64 assembly functions dataset from two source code corpora: C functions in The-Stack (Li et al., 2023) and AnghaBench (da Silva et al., 2021). We compile the C programs into executables using gcc with different optimization levels (i.e., 00, 01, 02 and 03), strip the executables to remove debug information, and disassemble them into X86-64 assembly code using objdump. We treat every function as a separate data point. Table 1 shows the number of C functions in the two original datasets, and the number of X86-64 assembly functions we collected from them.

We perform certain normalization on the assembly functions: (1) removing all the “%” and comments, (2) adding whitespace around “,”, “(”, “)”, (3) converting all the hexadecimal numbers to decimal numbers, and (4) replacing the address of each instruction with special labels (e.g., replacing “0” and “4” in Figure 1 (b) with “[INST-1]” and “[INST-2]”) placing at the end of each instruction. More details are in Appendix A.1.

3.2 HIERARCHICAL SELF-ATTENTION

Nova uses hierarchical self-attention that is specially designed to learn the *low-information-density* semantics in the *long* sequence of assembly code. Specifically, Nova learns the assembly code in an hierarchical way by providing a modified attention mask. Different from standard token-level attentions (Vaswani et al., 2017; Radford & Narasimhan, 2018; Radford et al., 2019; Brown et al., 2020), our hierarchical self-attention contains three categories at different levels of granularity.

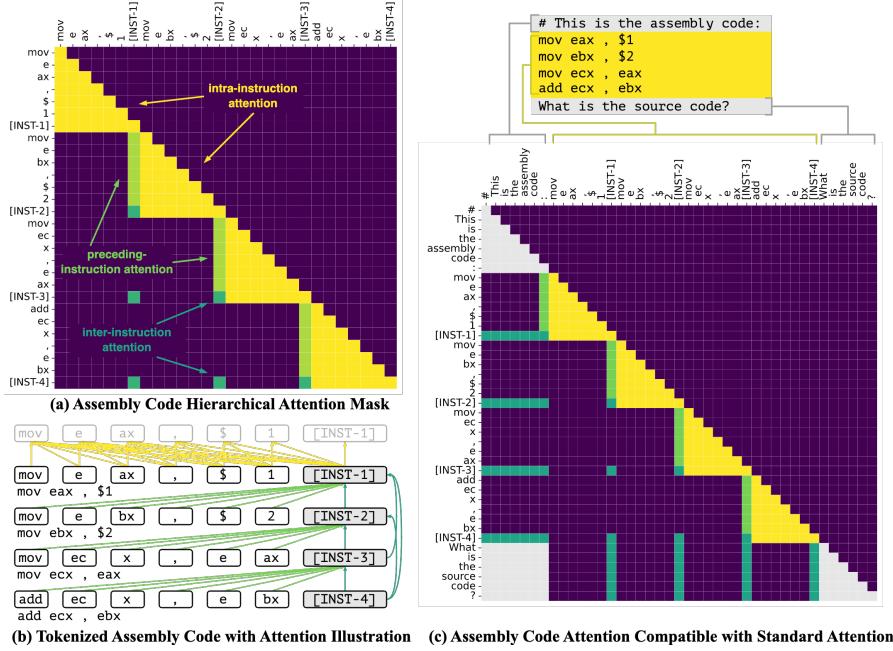


Figure 3: Design of Nova’s hierarchical attention for assembly code

(1) Intra-Instruction Attention: Due to the low information density in assembly, intra-instruction attention is designed to capture the summary of every instruction, which is the standard causal attention but limited to tokens of each instruction (the yellow part in Figures 3) (a) and (b). Tokens in different instructions have no attention weights. The “[INST]” label at the end of the instruction has attention to all the tokens in the instruction and thus captures the semantics of the entire instruction (e.g., “[INST-1]” captures the semantics of “mov eax, \$1”).

(2) Preceding-Instruction Attention: In addition to the local semantics of each instruction, the use of assembly instructions (such as the choice of registers) depends on the context. For example, after

the first instruction “`mov eax, $1`”, the second instruction should not reuse “`eax`” to store another value “`$2`” immediately. To capture such context, the preceding-instruction attention enables each token in an instruction to have attention to the “[INST]” label of the preceding instruction (the **light green** part in Figures 3 (a) and (b)).

(3) Inter-Instruction Attention: To understand function semantics (i.e., functionality), which lies in the dependencies across different instructions, the inter-instruction attention is designed to let the “[INST]” label of each instruction have attention to all the labels of previous instructions. For example, “[INST-4]” has attention to “[INST-1]”, “[INST-2]”, and “[INST-3]” (the **dark green** part in Figures 3 (a) and (b)). The inter-instruction attention is only enabled for “[INST]” labels, as they represent the semantics of each instruction.

To sum up, the hierarchical self-attention splits assembly code semantics into three levels: intra-instruction attention captures instruction summaries, preceding-instruction attention provides context from the preceding instruction, and inter-instruction attention models long dependencies across instructions using “[INST]” tokens that contain the instruction summary. Figure 3 (c) highlights the compatibility of Nova’s hierarchical attention with standard self-attention for text and source code. Leveraging the proven performance of standard self-attention in existing LLMs, we retain the causal attention mask within and across chunks of text or source code (shown in light grey in Figure 3 (c)). Cross-attention between text, source code, and assembly is restricted to “[INST]” tokens, which encapsulate assembly instruction summaries.

3.3 CONTRASTIVE LEARNING

The syntax gap between assembly code and source code, and syntax diversity between differently-optimized assembly code make LLMs struggle to distinguish the semantics behind the syntax. Nova adopts contrastive learning technique (Gao et al., 2021) during pre-training to train LLMs to encode assembly code meaningfully w.r.t semantics. The standard pre-training objective is language modeling by minimizing the negative likelihood of code in the pre-training corpus (Radford & Narasimhan, 2018), notated as L_{lm} . In addition, Nova is pre-trained with two new objectives, L_{fcl} for functionality contrastive learning and L_{ocl} for optimization contrastive learning.

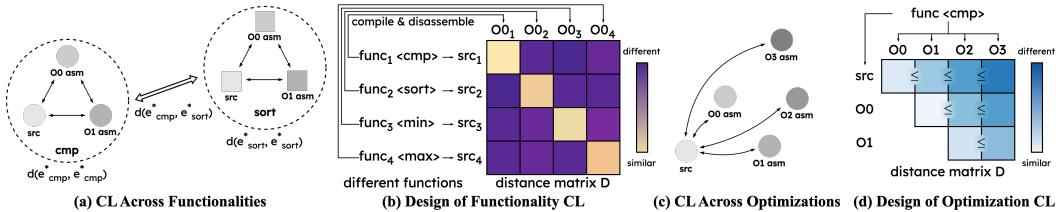


Figure 4: Design of functionality and optimization contrastive learning (CL). “asm” denotes assembly.

Functionality CL: Functionality CL trains Nova to focus more on the functionalities of assembly code rather than the syntax. Code with the same functionality (assemblies from the same source code), should be encoded closer in the latent space. For instance, in Figure 4 (a), embeddings of source and assembly code of function “`cmp`” are closer to each other, and the same for function “`sort`”.

Nova is designed and implemented on decoder-only generative LLMs, and we refer the hidden states from the last transformer layer as embedding. For source code, we use the average of each token’s embedding as the source code function’s embedding. For assembly, we use the average of all the “[INST]” tokens’ embedding as the embedding of the assembly function, as each “[INST]” token is supposed to capture the semantics of that instruction by the design of our hierarchical self-attention.

Let e_f^s be the embedding of function f in s form ($s = -1$ for source code, and $s \in [0, 1, 2, 3]$ for 00 to 03 optimized assembly). For simplicity, let $S = [-1, 0, 1, 2, 3]$ be the domain of s . Functionality CL optimizes Nova’s embeddings to satisfy the constraint:

$$\forall f_i \in F, \max_{s, t \in S} (d(e_{f_i}^s, e_{f_i}^t)) < \min_{\substack{s, t \in S \\ f_j \neq f_i \in F}} (d(e_{f_i}^s, e_{f_j}^t))$$

, where d calculates the l_2 distance between two embeddings and F is the full set of functions in the training corpus.

The embeddings of a batch of functions, each represented in two different forms, can be optimized to satisfy these constraints. For the example in Figure 4 (b), there are two forms (source code and 00 assembly) of four functions. Once Nova encodes the batch of source code and assembly functions, we calculate the distance matrix $\{D_{ij}\}_{f_i, f_j \in F} = \{d(e_{f_i}^s, e_{f_j}^t)\}$, and minimize the loss:

$$L_{fcl} = -\log \sum_{s, t \in S} \sum_{f_i \in F} \left(1 - \frac{\exp(d(e_{f_i}^s, e_{f_i}^t))}{\sum_{f_j \in F} \exp(d(e_{f_i}^s, e_{f_j}^t))} \right)$$

This objective minimizes the distance between the embeddings of the same function, which is the diagonal in the distance matrix. In practice, this loss is computed and back-propagated for each batch of functions. Given a batch size of 64, F represents a set of 64 unique functions in the batch.

Optimization CL: LLMs can be confused if being asked to directly connect a source code function to its 03-optimized assembly, due to their dramatically different syntax. Such a huge gap can be filled by learning how the source code is transformed to 00, 01, 02 and eventually to 03 assembly, as the optimization levels are *ordered*. Higher-level optimization applies a super-set of optimization rules compared to lower-level optimization.

Nova learns such order with the optimization CL objective, encoding differently-optimized assembly code orderly. Optimization CL optimizes Nova with the constraint: the more optimizations applied, the larger the difference between embeddings of optimized and unoptimized code. For instance, Figure 4 (c) and (d) illustrate that for the same function “`cmp`”, the distance between source code and assembly increases when the optimization level increases. Formally, optimization CL minimizes the following loss:

$$L_{ocl} = \sum_{f \in F} \sum_{s < t_1 < t_2 \in S} \max(0, d(e_f^s, e_f^{t_1}) - d(e_f^s, e_f^{t_2}))$$

Overall, the final training loss combines the three: $L = L_{lm} + \lambda(L_{fcl} + L_{ocl})$, where λ is set to 0.1 to balance the losses in this work.

3.4 TASK 1: BINARY CODE DECOMPILATION

Binary code decompilation (BCD) helps developers to understand binary code by recovering binary code into more readable high-level source code (e.g., C programs) (Fu et al., 2019; Liang et al., 2021; Armengol-Estabé et al., 2024; Tan et al., 2024). The input to the model for BCD is formatted as an instruction prompt (notated by \mathbf{p}): # This is the assembly code with {opt} optimization: {asm}, where “`opt`” is the optimization-level applied to the assembly and “`asm`” is the assembly code to decompile. Nova is fine-tuned to generate the expected source code function `src` following the instruction prompt. The fine-tuning objective is minimizing the loss: $L_{bcd} = -\log P(\mathbf{src}|\mathbf{p})$.

3.5 TASK 2: BINARY CODE SIMILARITY DETECTION

Binary code similarity detection (BCSD) aims to measure the similarity between two binary code snippets (Wang et al., 2022; Su et al., 2024), which is the foundation of various applications such as plagiarism detection (Luo et al., 2014; Sæbjørnsen et al., 2009) and vulnerability detection (David & Yahav, 2014; David et al., 2018; 2017; 2016).

A widely used setting is taking a query assembly of the function f^q that is compiled with one optimization level (denoted by s), and a pool of candidate assembly of K (e.g., 50, 100, etc.) functions (notated by f_i^p , $1 \leq i \leq K$) compiled with a different optimization level (denoted by $t \neq s$). There exists a unique candidate assembly coming from the same source code as the query ($\exists! 1 \leq i \leq K, f_i^p = f^q$, called the positive candidate). Nova is fine-tuned to encode these binaries, so that the positive candidate has the highest similarity with the query assembly among the pool. The learning objective is as follows:

$$L_{BCSD} = -\log \sum_{1 \leq i \leq K}^{f^q := f_i^p} \left(1 - \frac{\exp \left(d(e_{f^q}^s, e_{f_i^p}^t) \right)}{\sum_{1 \leq j \leq K} \exp \left(d(e_{f^q}^s, e_{f_j^p}^t) \right)} \right)$$

We follow previous work (Su et al., 2024) to let s be 00-assembly and t be 03-assembly, which is the hardest setting.

4 EXPERIMENTAL SETUP

This section describes the setup of pre-training and fine-tuning of Nova, as well as the existing baselines we compare Nova with, and the evaluation metrics we used in the two downstream tasks. Appendix A.2 contains additional details such as training hyper-parameters, and evaluation setup.

4.1 PRE-TRAINING

We use the C and X86-64 assembly functions collected from AnghaBench and The-Stack for pre-training. We pre-train Nova starting from DeepSeek-Coder (Guo et al., 2024), and the hierarchical attention is applied on half of the attention heads to balance between its effectiveness and the existing knowledge in the standard attention layers (Justified in Appendix A.3). Nova is pre-trained with language modeling for one epoch, followed by contrastive learning objectives for another epoch.

4.2 FINE-TUNING FOR BINARY CODE DECOMPILATION

Training Data: We sample (due to computation resource limitation) 2.16M assembly-to-source-code pairs (0.338B tokens) from the pre-training corpus to build the BCD fine-tuning data.

Test Data: We use HumanEval-Decompile (Tan et al., 2024) as the test benchmark, which was not used in training. HumanEval-Decompile is derived from the C language adaptation of the HumanEval (Chen et al., 2021) benchmark and contains 164 C functions, each compiled with 00 – 03 optimization flags and disassembled into X86-64 assembly.

Baselines: Nova is compared with existing SOTA LLM4Decompile (Tan et al., 2024), Meta LLM-Compiler (Cummins et al., 2024), other open-sourced general code LLMs (Rozière et al., 2023; Lozhkov et al., 2024; Guo et al., 2024; Hui et al., 2024; Mishra et al., 2024; Guo et al., 2023), and commercial LLMs GPT-3.5-Turbo and GPT-4o). LLM4Decompile trains DeepSeekCoder using the same AnghaBench corpus for binary decompilation. Meta LLMCompiler trains CodeLlama models using LLVM IRs, X86, and ARM assembly code to optimize and translate binary code.

Evaluation: We let each model sample 20 decompilations per assembly function, using the temperature of 0.2 and top-p of 0.95 (Chen et al., 2021). Except for LLM4Decompile and Nova that are fine-tuned for binary code decompilation, we provide all other baselines with three-shot examples for few-shot learning (Brown et al., 2020). The decompilations are executed with the test cases to verify the functional correctness. Finally, Pass@1 and Pass@10 (Chen et al., 2021) are reported.

4.3 FINE-TUNING FOR BINARY CODE SIMILARITY DETECTION

Training Data: To compare Nova with existing works on BCSD fairly (Wang et al., 2022; Su et al., 2024), we use the same dataset, BinaryCorp-3M (Wang et al., 2022), as the fine-tuning data for BCSD, which contains the 00 and 03 assembly of 224,606 functions.

Test Data: Following existing work (Su et al., 2024; Xu et al., 2023a), we use real-world benchmarks, Binutils, Curl, ImageMagick, SQLite, OpenSSL, and Putty, as the test benchmarks, which are nonexistent in the training data.

Baselines: Nova is compared with jTrans (Wang et al., 2022), DiEmph (Xu et al., 2023a) and CodeArt (Su et al., 2024). jTrans is a Transformer (Vaswani et al., 2017) encoder trained on binaries with masked token prediction and jump target prediction tasks. DiEmph uses an instruction deemphasis technique to prevent the model from learning instruction distribution biases introduced by

compilers. CodeArt proposes a regularized attention mask for encoder models to capture instructional semantics and data dependencies.

Evaluation: We randomly sample $K = 50, 100, 200, 500$ source code functions from each project, compile them into binaries with `00` and `03` optimization flags, and disassemble them into X86-64 assemblies. BCSD techniques encode these assemblies into embeddings (Nova uses the average last-layer hidden states of all the “[INST]” tokens in an assembly as its embedding). Then each `00` assembly is used as the query to calculate their similarity with the K `03` candidate assemblies. Metric Recall@1 is reported as the ratio of queries for which the candidate from the same source code has the highest similarity among all the candidates.

5 RESULTS

5.1 BINARY CODE DECOMPILATION

Comparison with SOTA Techniques: Table 2 shows the Pass@1 and Pass@10 of the decompiled code from assemblies on HumanEval-Decompile. The results are grouped by optimization level (i.e., the benchmark contains 164 assemblies of each optimization level), and the average is also reported.

Table 2: Nova’s Pass@K and comparison with existing techniques on HumanEval-Decompile.

Techniques	Pass@1					Pass@10				
	O0	O1	O2	O3	Avg.	O0	O1	O2	O3	Avg.
CodeLlama-7B	6.95	3.81	4.54	3.78	4.77	8.53	5.97	7.34	5.17	6.75
StarCoder2-7B	6.31	4.33	5.64	5.95	5.56	8.77	5.18	6.09	7.17	6.80
DeepSeekCoder-7B	9.63	7.56	7.41	6.68	7.82	13.60	11.38	11.52	9.44	11.49
Qwen-2.5-Coder-7B	4.76	5.79	5.58	5.27	5.35	6.34	7.69	6.56	5.79	6.60
LLMCompiler-7B	5.95	5.85	5.55	5.82	5.79	7.01	7.31	7.47	7.01	7.20
GPT-3.5-Turbo	7.41	6.13	4.33	3.90	5.44	9.56	8.38	6.23	5.12	7.32
GPT-4o	21.34	18.29	14.48	13.05	16.79	29.94	26.74	21.42	19.88	24.50
LLM4Decompile-1.3B	15.30	8.26	9.36	8.38	10.33	21.79	15.23	16.17	13.70	16.72
Nova-1.3B	37.53	21.71	22.68	18.75	25.17	49.38	34.84	36.95	32.03	38.30
LLM4Decompile-6.7B	29.97	19.05	20.46	18.32	21.95	40.40	27.75	28.85	28.51	31.38
Nova-6.7B	48.78	30.58	30.85	27.23	34.36	57.47	47.45	43.03	39.68	46.91

Overall, Nova’s Pass@1 and Pass@10 are higher than all SOTA binary decompilation techniques and general LLMs with even smaller model sizes. Specifically, for each optimization level, Nova consistently decompiles more assemblies into source code correctly than the rest of the compared techniques. Note that Meta LLMCompiler is mainly designed for LLVM IR optimization, and thus is still incapable of assembly code decompilation.

With the same model size, Nova-1.3B outperforms LLM4Decompile-1.3B with a 14.84% higher averaged Pass@1, and a 21.58% higher Pass@10. Nova-6.7B outperforms LLM4Decompile-6.7B with a 12.41% higher averaged Pass@1, and a 15.53% higher Pass@10. When compared with GPT-4o, an order of magnitude larger model, Nova-1.3B produces an 8.38% higher Pass@1 and 13.80% higher Pass@10. Examples of Nova’s correct decompilation are provided in Appendix A.5.

Comparison with Techniques Handling Long Input: Nova’s hierarchical attention design targets to address the low information density and long input challenge of assembly code. There are other techniques that handles long input challenges in text and source code, with Granite-3B-Code-Base-128K and LongCoder being the most related ones.

Granite trains LLM on repository-level long inputs, which is an orthogonal approach with Nova’s approach (hierarchical attention and contrastive learning). We train Granite-3B-Code-128K with Nova’s approach, and Table 3 shows that Nova’s approach brings improvement to Granite over standard fine-tuning even if it has already been trained with long code data.

LongCoder combines window attention and global attention to learn long code input. We compare LongCoder’s attention design with Nova’s hierarchical attention design by replacing the hierarchical attention of Nova-1.3B with LongCoder’s attention design. Table 4 shows that Nova’s hierarchical attention is more effective in learning assembly code. Nova’s attention design considers the instruction-

Table 3: Nova’s approach brings improvement to LLM that has been trained with long input data.

Techniques	Pass@1					Pass@10				
	O0	O1	O2	O3	Avg.	O0	O1	O2	O3	Avg.
Granite (3B-Code-128K)	5.91	3.78	5.09	5.52	5.08	8.19	5.16	6.56	7.15	6.76
Granite + Standard Fine-Tuning	20.88	13.54	11.37	10.09	13.97	30.05	19.77	18.31	15.77	20.98
Granite + Nova’s Approaches	31.04	14.57	14.70	13.66	18.49	39.57	21.23	21.77	19.82	25.60

Table 4: Nova’s hierarchical attention is more effective on assembly code.

Techniques	Pass@1					Pass@10				
	O0	O1	O2	O3	Avg.	O0	O1	O2	O3	Avg.
Nova-1.3B (using LongCoder’s Attention)	34.59	19.07	19.72	17.34	22.68	42.19	32.37	32.86	29.04	34.12
Nova-1.3B	37.53	21.71	22.68	18.75	25.17	49.38	34.84	36.95	32.03	38.30

level local semantics and dependencies between different instructions, which fits better than fix-sized window attention to assembly code.

Ablation Study: We conduct an ablation study by comparing Nova-1.3B with the following models to show the effectiveness of contrastive learning objectives and hierarchical attention design:

- Nova_{-CL-HA} : Removing contrastive learning and hierarchical self-attention. This is simply training DeepSeekCoder-1.3B on the assembly corpus using language modeling. This can be viewed as our reproduction (retrain) of LLM4Decompile-1.3B using the same amount of data.
- Nova_{-HA} : Removing the hierarchical self-attention, training DeepSeekCoder-1.3B on the assembly corpus using both the language modeling and contrastive learning objectives.

Table 5 shows the results of the ablation study. Nova_{-CL-HA} produces an average Pass@1 of 15.78% and Pass@10 of 27.41%. With additional contrastive learning objectives, Nova_{-HA} improves the Pass@1 on all optimization levels over Nova_{-CL-HA} , showing a higher averaged Pass@1 and Pass@10. Further applying the hierarchical self-attention on Nova_{-HA} boosts the overall Pass@1 from 21.86% to 25.17%, and Pass@10 from 35.25% to 38.30%.

5.2 BINARY CODE SIMILARITY DETECTION

Tables 6, 7, 8 and 9 show the Recall@1 of Nova and existing BCSD techniques with pool size K of 50, 100, 200 and 500 on the six benchmarks. Underline indicates the best in each benchmark, while wave denotes the tied best (we only mark Nova-1.3B for clearer illustration).

Overall, Tables 6, 7, 8 and 9 show that *on average, Nova-1.3B and Nova-6.7B achieve the highest Recall@1 (in bold) under all four settings of K* . Nova-6.7B further outperforms Nova-1.3B and achieves the highest averaged Recall@1 under all four settings, ranking the ground-truth of 5%, 2%, 4%, and 3% more queries the most similar correspondingly compared to CodeArt. Nova-1.3B consistently outperforms existing techniques with higher Recall@1 when K is 50, 100, and 200, meaning it correctly ranks ground-truth of 3%, 1%, and 2% more queries as the most similar. Under the setting of $K = 500$, Nova-1.3B ties with CodeArt with the same highest Recall@1. When looking into each individual benchmark, Nova-1.3B always wins on the most benchmarks under different settings of pool size K . For instance, Nova-1.3B wins on four benchmarks while DiEmph only wins on SQLite when $K = 50$. We also conduct an ablation study on BCSD in Appendix A.6.

5.3 ANALYTIC EXPERIMENTS: HOW ARE NOVA’S EMBEDDINGS BETTER?

We use the widely-used t-SNE (van der Maaten & Hinton, 2008) to analyze and visualize high-dimensional embeddings. We randomly sample seven coding problems from HumanEval-Decompile (task_id 19, 32, 34, 63, 119, 128, 143), encode the 00 – 03 assemblies by Nova_{-CL-HA} and Nova-1.3B. Figure 5 shows the embeddings that are visualized under the first two principal components. Each color represents one task, and 00 – 03 assemblies are marked by \bigcirc , \bigtriangledown , \triangle , and \square .

Compared with Nova_{-CL-HA} (Figure 5 (a)), Nova_{-HA} (Figure 5 (b)) including contrastive learning objectives in the pre-training, can separate the embeddings of assemblies with different functionalities better. Nova_{-HA} clearly encode “Task 143” (orange points) away from the others. Yet, Nova’s

Table 5: Ablation study of Nova-1.3B on HumanEval-Decompile.

Techniques	Pass@1					Pass@10				
	O0	O1	O2	O3	Avg.	O0	O1	O2	O3	Avg.
LLM4Decompile-1.3B	15.30	8.26	9.36	8.38	10.33	21.79	15.23	16.17	13.70	16.72
Nova_{-CL-HA}	20.73	16.16	15.03	11.19	15.78	33.55	28.12	26.96	21.01	27.41
Nova_{-HA}	30.58	19.88	20.58	16.40	21.86	44.75	33.13	33.31	29.82	35.25
Nova	37.53	21.71	22.68	18.75	25.17	49.38	34.84	36.95	32.03	38.30

Table 6: Recall@1 on BCSD with $K = 50$

Benchmarks	jTrans	DiEmph	CodeArt	Nova-1.3B	Nova-6.7B
Binutils	0.68	0.80	0.84	<u>0.87</u>	0.89
Curl	0.72	0.84	0.86	<u>0.89</u>	0.94
ImageMagick	0.53	0.71	0.78	<u>0.86</u>	0.90
SQLite	0.73	<u>0.79</u>	0.78	<u>0.77</u>	0.78
OpenSSL	0.70	0.83	0.88	<u>0.90</u>	0.92
Putty	0.63	<u>0.72</u>	0.69	<u>0.72</u>	0.71
Avg.	0.67	0.78	0.81	0.84	0.86

Table 8: Recall@1 on BCSD with $K = 200$

Benchmarks	jTrans	DiEmph	CodeArt	Nova-1.3B	Nova-6.7B
Binutils	0.51	0.64	<u>0.74</u>	0.73	0.73
Curl	0.57	0.77	0.78	<u>0.83</u>	0.84
ImageMagick	0.39	0.51	0.67	<u>0.73</u>	0.75
SQLite	0.56	0.65	<u>0.68</u>	<u>0.68</u>	0.69
OpenSSL	0.54	0.71	0.82	<u>0.84</u>	0.88
Putty	0.49	<u>0.58</u>	0.55	0.55	0.58
Avg.	0.51	0.64	0.71	0.73	0.75

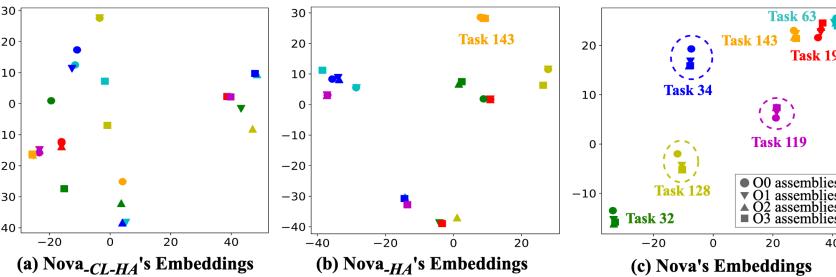
Table 7: Recall@1 on BCSD with $K = 100$

Benchmarks	jTrans	DiEmph	CodeArt	Nova-1.3B	Nova-6.7B
Binutils	0.60	0.63	<u>0.81</u>	0.79	0.79
Curl	0.63	0.80	<u>0.82</u>	<u>0.86</u>	0.88
ImageMagick	0.54	0.71	0.76	<u>0.79</u>	0.81
SQLite	0.62	0.72	<u>0.74</u>	0.73	0.72
OpenSSL	0.60	0.80	0.87	<u>0.88</u>	0.90
Putty	0.58	0.64	0.64	<u>0.65</u>	0.64
Avg.	0.60	0.72	0.77	0.78	0.79

Table 9: Recall@1 on BCSD with $K = 500$

Benchmarks	jTrans	DiEmph	CodeArt	Nova-1.3B	Nova-6.7B
Binutils	0.40	0.57	<u>0.70</u>	0.65	0.67
Curl	0.43	0.62	0.69	<u>0.73</u>	0.76
ImageMagick	0.25	0.42	0.58	<u>0.61</u>	0.65
SQLite	0.43	0.59	<u>0.62</u>	0.59	0.62
OpenSSL	0.43	0.61	0.76	<u>0.78</u>	0.82
Putty	0.38	<u>0.50</u>	0.49	0.47	0.51
Avg.	0.39	0.55	0.64	0.64	0.67

(Figure 5 (c)) embeddings group the assemblies by functionalities more precisely than Nova_{-HA} , suggesting that hierarchical attention enhances the training of contrastive learning objectives to learn more effective encoding. Visualization using a different approach, PCA, is shown in Appendix A.7. Analytic experiments on Nova’s hierarchical attention is shown in Appendix A.8.

Figure 5: t-SNE analysis of embeddings calculated by Nova_{-CL-HA} , Nova_{-HA} , and Nova.

6 CONCLUSION

This work presents Nova, a generative foundation LLM for assembly code that introduces two key innovations—hierarchical attention and contrastive learning—to tackle the unique challenges of assembly code understanding. Nova builds upon a source code LLM and undergoes further pre-training on approximately 4.3 million collected assembly functions. We fine-tune and evaluate Nova on two downstream tasks: binary code decompilation and binary code similarity detection. Nova achieves up to 14.84 – 21.58% (absolute percentage point improvement) higher Pass@1 and Pass@10 over existing methods in binary code decompilation and up to a 6.17% higher Recall@1 in binary code similarity detection. Looking forward, we believe that the proposed hierarchical attention and contrastive learning methods hold promise for enhancing foundation models in both source code and natural language domains, which we leave as future work.

ACKNOWLEDGMENTS

This research was supported in part by NSF 1901242 and 2006688, a CFI fund, and J.P. Morgan AI Faculty Research Awards. Any opinions, findings, and conclusions in this paper are those of the authors only and do not necessarily reflect the views of our sponsors.

REFERENCES

Simone Aonzo, Yufei Han, Alessandro Mantovani, and Davide Balzarotti. Humans vs. Machines in Malware Classification. In *32nd USENIX Security Symposium (USENIX Security 23)*, pp. 1145–1162, Anaheim, CA, 2023. USENIX Association. ISBN 978-1-939133-37-3. URL <https://www.usenix.org/conference/usenixsecurity23/presentation/aonzo>.

Jordi Armengol-Estabé, Jackson Woodruff, Chris Cummins, and Michael F. P. O’Boyle. SLaDe: A Portable Small Language Model Decompiler for Optimized Assembly, 2024.

Tom B. Brown, Benjamin Mann, Nick Ryder, Melanie Subbiah, Jared Kaplan, Prafulla Dhariwal, Arvind Neelakantan, Pranav Shyam, Girish Sastry, Amanda Askell, Sandhini Agarwal, Ariel Herbert-Voss, Gretchen Krueger, Tom Henighan, Rewon Child, Aditya Ramesh, Daniel M. Ziegler, Jeffrey Wu, Clemens Winter, Christopher Hesse, Mark Chen, Eric Sigler, Mateusz Litwin, Scott Gray, Benjamin Chess, Jack Clark, Christopher Berner, Sam McCandlish, Alec Radford, Ilya Sutskever, and Dario Amodei. Language Models are Few-Shot Learners. *CoRR*, abs/2005.14165, 2020. URL <https://arxiv.org/abs/2005.14165>.

Martim Carbone, Weidong Cui, Long Lu, Wenke Lee, Marcus Peinado, and Xuxian Jiang. Mapping kernel objects to enable systematic integrity checking. In *Proceedings of the 16th ACM Conference on Computer and Communications Security*, CCS ’09, pp. 555–565, New York, NY, USA, 2009. Association for Computing Machinery. ISBN 9781605588940. doi: 10.1145/1653662.1653729. URL <https://doi.org/10.1145/1653662.1653729>.

Nicholas Carlini, Antonio Barresi, Mathias Payer, David Wagner, and Thomas R. Gross. Control-Flow Bending: On the Effectiveness of Control-Flow Integrity. In *24th USENIX Security Symposium (USENIX Security 15)*, pp. 161–176, Washington, D.C., 2015. USENIX Association. ISBN 978-1-939133-11-3. URL <https://www.usenix.org/conference/usenixsecurity15/technical-sessions/presentation/carlini>.

Lei Chai and Ming Li. Pyramid attention for source code summarization. In *Proceedings of the 36th International Conference on Neural Information Processing Systems*, NIPS ’22, Red Hook, NY, USA, 2024. Curran Associates Inc. ISBN 9781713871088.

Angelica Chen, Jérémie Scheurer, Tomasz Korbak, Jon Ander Campos, Jun Shern Chan, Samuel R. Bowman, Kyunghyun Cho, and Ethan Perez. Improving Code Generation by Training with Natural Language Feedback, 2023.

Bei Chen, Fengji Zhang, Anh Nguyen, Daoguang Zan, Zeqi Lin, Jian-Guang Lou, and Weizhu Chen. CodeT: Code Generation with Generated Tests, 2022a. URL <https://arxiv.org/abs/2207.10397>.

Ligeng Chen, Zhongling He, Hao Wu, Fengyuan Xu, Yi Qian, and Bing Mao. DICoMP: Lightweight Data-Driven Inference of Binary Compiler Provenance with High Accuracy. In *2022 IEEE International Conference on Software Analysis, Evolution and Reengineering (SANER)*, pp. 112–122, 2022b. doi: 10.1109/SANER53432.2022.00025.

Mark Chen, Jerry Tworek, Heewoo Jun, Qiming Yuan, Henrique Ponde de Oliveira Pinto, Jared Kaplan, Harrison Edwards, Yuri Burda, Nicholas Joseph, Greg Brockman, Alex Ray, Raul Puri, Gretchen Krueger, Michael Petrov, Heidy Khlaaf, Girish Sastry, Pamela Mishkin, Brooke Chan, Scott Gray, Nick Ryder, Mikhail Pavlov, Alethea Power, Lukasz Kaiser, Mohammad Bavarian, Clemens Winter, Philippe Tillet, Felipe Petroski Such, Dave Cummings, Matthias Plappert, Fotios Chantzis, Elizabeth Barnes, Ariel Herbert-Voss, William Hebgen Guss, Alex Nichol, Alex Paino, Nikolas Tezak, Jie Tang, Igor Babuschkin, Suchir Balaji, Shantanu Jain, William Saunders, Christopher Hesse, Andrew N. Carr, Jan Leike, Joshua Achiam, Vedant Misra, Evan Morikawa,

Alec Radford, Matthew Knight, Miles Brundage, Mira Murati, Katie Mayer, Peter Welinder, Bob McGrew, Dario Amodei, Sam McCandlish, Ilya Sutskever, and Wojciech Zaremba. Evaluating Large Language Models Trained on Code. *CoRR*, abs/2107.03374, 2021. URL <https://arxiv.org/abs/2107.03374>.

Qibin Chen, Jeremy Lacomis, Edward J. Schwartz, Claire Le Goues, Graham Neubig, and Bogdan Vasilescu. Augmenting Decomplier Output with Learned Variable Names and Types. In *31st USENIX Security Symposium (USENIX Security 22)*, pp. 4327–4343, Boston, MA, aug 2022c. USENIX Association. ISBN 978-1-939133-31-1. URL <https://www.usenix.org/conference/usenixsecurity22/presentation/chen-qibin>.

Simin Chen, Hamed Khanpour, Cong Liu, and Wei Yang. Learning to Reverse DNNs from AI Programs Automatically, 2022d. URL <https://arxiv.org/abs/2205.10364>.

Kevin Clark, Urvashi Khandelwal, Omer Levy, and Christopher D. Manning. What Does BERT Look at? An Analysis of BERT’s Attention. In Tal Linzen, Grzegorz Chrupała, Yonatan Belinkov, and Dieuwke Hupkes (eds.), *Proceedings of the 2019 ACL Workshop BlackboxNLP: Analyzing and Interpreting Neural Networks for NLP*, pp. 276–286, Florence, Italy, August 2019. Association for Computational Linguistics. doi: 10.18653/v1/W19-4828. URL <https://aclanthology.org/W19-4828>.

Chris Cummins, Volker Seeker, Dejan Grubisic, Baptiste Roziere, Jonas Gehring, Gabriel Synnaeve, and Hugh Leather. Meta Large Language Model Compiler: Foundation Models of Compiler Optimization, 2024. URL <https://arxiv.org/abs/2407.02524>.

Anderson Faustino da Silva, Bruno Conde Kind, José Wesley de Souza Magalhães, Jerônimo Nunes Rocha, Breno Campos Ferreira Guimarães, and Fernando Magno Quinão Pereira. ANGHABENCH: A Suite with One Million Compilable C Benchmarks for Code-Size Reduction. In *2021 IEEE/ACM International Symposium on Code Generation and Optimization (CGO)*, pp. 378–390, 2021. doi: 10.1109/CGO51591.2021.9370322.

Yaniv David and Eran Yahav. Tracelet-Based Code Search in Executables. In *Proceedings of the 35th ACM SIGPLAN Conference on Programming Language Design and Implementation*, PLDI ’14, pp. 349–360, New York, NY, USA, 2014. Association for Computing Machinery. ISBN 9781450327848. doi: 10.1145/2594291.2594343. URL <https://doi.org/10.1145/2594291.2594343>.

Yaniv David, Nimrod Partush, and Eran Yahav. Statistical Similarity of Binaries. In *Proceedings of the 37th ACM SIGPLAN Conference on Programming Language Design and Implementation*, PLDI ’16, pp. 266–280, New York, NY, USA, 2016. Association for Computing Machinery. ISBN 9781450342612. doi: 10.1145/2908080.2908126. URL <https://doi.org/10.1145/2908080.2908126>.

Yaniv David, Nimrod Partush, and Eran Yahav. Similarity of Binaries through Re-Optimization. *SIGPLAN Not.*, 52(6):79–94, jun 2017. ISSN 0362-1340. doi: 10.1145/3140587.3062387. URL <https://doi.org/10.1145/3140587.3062387>.

Yaniv David, Nimrod Partush, and Eran Yahav. FirmUp: Precise Static Detection of Common Vulnerabilities in Firmware. *SIGPLAN Not.*, 53(2):392–404, mar 2018. ISSN 0362-1340. doi: 10.1145/3296957.3177157. URL <https://doi.org/10.1145/3296957.3177157>.

Steven H. H. Ding, Benjamin C. M. Fung, and Philippe Charland. Asm2Vec: Boosting Static Representation Robustness for Binary Clone Search against Code Obfuscation and Compiler Optimization. In *2019 IEEE Symposium on Security and Privacy (SP)*, pp. 472–489, 2019. doi: 10.1109/SP.2019.00003.

Yue Duan, Xuezixiang Li, Jinghan Wang, and Heng Yin. DeepBinDiff: Learning Program-Wide Code Representations for Binary Differing. 01 2020. doi: 10.14722/ndss.2020.24311.

Daniel Fried, Armen Aghajanyan, Jessy Lin, Sida Wang, Eric Wallace, Freda Shi, Ruiqi Zhong, Wentau Yih, Luke Zettlemoyer, and Mike Lewis. InCoder: A Generative Model for Code Infilling and Synthesis, 2023.

Cheng Fu, Huili Chen, Haolan Liu, Xinyun Chen, Yuandong Tian, Farinaz Koushanfar, and Jishen Zhao. Coda: An End-to-End Neural Program Decompiler. In H. Wallach, H. Larochelle, A. Beygelzimer, F. d’Alché-Buc, E. Fox, and R. Garnett (eds.), *Advances in Neural Information Processing Systems*, volume 32. Curran Associates, Inc., 2019. URL https://proceedings.neurips.cc/paper_files/paper/2019/file/093b60fd0557804c8ba0cbf1453da22f-Paper.pdf.

Tianyu Gao, Xingcheng Yao, and Danqi Chen. SimCSE: Simple Contrastive Learning of Sentence Embeddings. In *Proceedings of the 2021 Conference on Empirical Methods in Natural Language Processing*, pp. 6894–6910, Online and Punta Cana, Dominican Republic, November 2021. Association for Computational Linguistics. doi: 10.18653/v1/2021.emnlp-main.552. URL <https://aclanthology.org/2021.emnlp-main.552>.

Emre Güler, Cornelius Aschermann, Ali Abbasi, and Thorsten Holz. AntiFuzz: Impeding Fuzzing Audits of Binary Executables. In *28th USENIX Security Symposium (USENIX Security 19)*, pp. 1931–1947, Santa Clara, CA, 2019. USENIX Association. ISBN 978-1-939133-06-9. URL <https://www.usenix.org/conference/usenixsecurity19/presentation/guler>.

Daya Guo, Canwen Xu, Nan Duan, Jian Yin, and Julian McAuley. LongCoder: a long-range pre-trained language model for code completion. In *Proceedings of the 40th International Conference on Machine Learning*, ICML’23. JMLR.org, 2023.

Daya Guo, Qihao Zhu, Dejian Yang, Zhenda Xie, Kai Dong, Wentao Zhang, Guanting Chen, Xiao Bi, Y. Wu, Y. K. Li, Fulí Luo, Yingfei Xiong, and Wenfeng Liang. DeepSeek-Coder: When the Large Language Model Meets Programming – The Rise of Code Intelligence, 2024.

Jingxuan He and Martin Vechev. Large Language Models for Code: Security Hardening and Adversarial Testing. *CoRR*, abs/2302.05319, 2023. URL <https://arxiv.org/abs/2302.05319>.

Jingxuan He, Pesho Ivanov, Petar Tsankov, Veselin Raychev, and Martin Vechev. Debin: Predicting Debug Information in Stripped Binaries. In *Proceedings of the 2018 ACM SIGSAC Conference on Computer and Communications Security*, CCS ’18, pp. 1667–1680, New York, NY, USA, 2018. Association for Computing Machinery. ISBN 9781450356930. doi: 10.1145/3243734.3243866. URL <https://doi.org/10.1145/3243734.3243866>.

Iman Hosseini and Brendan Dolan-Gavitt. Beyond the C: Retargetable Decompilation using Neural Machine Translation. In *Proceedings 2022 Workshop on Binary Analysis Research*, BAR 2022. Internet Society, 2022. doi: 10.14722/bar.2022.23009. URL <http://dx.doi.org/10.14722/bar.2022.23009>.

Yunpeng Huang, Jingwei Xu, Junyu Lai, Zixu Jiang, Taolue Chen, Zenan Li, Yuan Yao, Xiaoxing Ma, Lijuan Yang, Hao Chen, Shupeng Li, and Penghao Zhao. Advancing Transformer Architecture in Long-Context Large Language Models: A Comprehensive Survey, 2024. URL <https://arxiv.org/abs/2311.12351>.

Bin Yuan Hui, Jian Yang, Zeyu Cui, Jiaxi Yang, Dayiheng Liu, Lei Zhang, Tianyu Liu, Jiajun Zhang, Bowen Yu, Kai Dang, An Yang, Rui Men, Fei Huang, Xingzhang Ren, Xuancheng Ren, Jingren Zhou, and Junyang Lin. Qwen2.5-Coder Technical Report. *arXiv preprint arXiv:2409.12186*, 2024.

Nan Jiang, Kevin Liu, Thibaud Lutellier, and Lin Tan. Impact of Code Language Models on Automated Program Repair. In *Proceedings of the 45th International Conference on Software Engineering*, ICSE ’23, pp. 1430–1442. IEEE Press, 2023. ISBN 9781665457019. doi: 10.1109/ICSE48619.2023.00125. URL <https://doi.org/10.1109/ICSE48619.2023.00125>.

Jeremy Lacomis, Pengcheng Yin, Edward J. Schwartz, Miltiadis Allamanis, Claire Le Goues, Graham Neubig, and Bogdan Vasilescu. DIRE: a neural approach to decompiled identifier naming. In *Proceedings of the 34th IEEE/ACM International Conference on Automated Software Engineering*, ASE ’19, pp. 628–639. IEEE Press, 2020. ISBN 9781728125084. doi: 10.1109/ASE.2019.00064. URL <https://doi.org/10.1109/ASE.2019.00064>.

Hung Le, Yue Wang, Akhilesh Deepak Gotmare, Silvio Savarese, and Steven C.H. Hoi. CodeRL: Mastering Code Generation through Pretrained Models and Deep Reinforcement Learning. *arXiv preprint*, abs/2207.01780, 2022.

Mike Lewis, Yinhan Liu, Naman Goyal, Marjan Ghazvininejad, Abdelrahman Mohamed, Omer Levy, Ves Stoyanov, and Luke Zettlemoyer. BART: Denoising Sequence-to-Sequence Pre-training for Natural Language Generation, Translation, and Comprehension, 2019.

Raymond Li, Loubna Ben Allal, Yangtian Zi, Niklas Muennighoff, Denis Kocetkov, Chenghao Mou, Marc Marone, Christopher Akiki, Jia Li, Jenny Chim, Qian Liu, Evgenii Zhettonozhskii, Terry Yue Zhuo, Thomas Wang, Olivier Dehaene, Mishig Davaadorj, Joel Lamy-Poirier, João Monteiro, Oleh Shliazhko, Nicolas Gontier, Nicholas Meade, Armel Zebaze, Ming-Ho Yee, Logesh Kumar Umapathi, Jian Zhu, Benjamin Lipkin, Muhtasham Oblokulov, Zhiruo Wang, Rudra Murthy, Jason Stillerman, Siva Sankalp Patel, Dmitry Abulkhanov, Marco Zocca, Manan Dey, Zhihan Zhang, Nour Fahmy, Urvashi Bhattacharyya, Wenhao Yu, Swayam Singh, Sasha Luccioni, Paulo Villegas, Maxim Kunakov, Fedor Zhdanov, Manuel Romero, Tony Lee, Nadav Timor, Jennifer Ding, Claire Schlesinger, Hailey Schoelkopf, Jan Ebert, Tri Dao, Mayank Mishra, Alex Gu, Jennifer Robinson, Carolyn Jane Anderson, Brendan Dolan-Gavitt, Danish Contractor, Siva Reddy, Daniel Fried, Dzmitry Bahdanau, Yacine Jernite, Carlos Muñoz Ferrandis, Sean Hughes, Thomas Wolf, Arjun Guha, Leandro von Werra, and Harm de Vries. StarCoder: may the source be with you!, 2023.

Ruigang Liang, Ying Cao, Peiwei Hu, and Kai Chen. Neutron: an attention-based neural decompiler. *Cybersecurity*, 4(1):5, 2021. ISSN 2523-3246. doi: 10.1186/s42400-021-00070-0. URL <https://doi.org/10.1186/s42400-021-00070-0>.

Jiate Liu, Yiqin Zhu, Kaiwen Xiao, Qiang Fu, Xiao Han, Wei Yang, and Deheng Ye. RLTf: Reinforcement Learning from Unit Test Feedback, 2023a.

Zhibo Liu, Yuanyuan Yuan, Shuai Wang, Xiaofei Xie, and Lei Ma. Decompiling x86 deep neural network executables. In *Proceedings of the 32nd USENIX Conference on Security Symposium, SEC '23*, USA, 2023b. USENIX Association. ISBN 978-1-939133-37-3.

Anton Lozhkov, Raymond Li, Loubna Ben Allal, Federico Cassano, Joel Lamy-Poirier, Nouamane Tazi, Ao Tang, Dmytro Pykhtar, Jiawei Liu, Yuxiang Wei, Tianyang Liu, Max Tian, Denis Kocetkov, Arthur Zucker, Younes Belkada, Zijian Wang, Qian Liu, Dmitry Abulkhanov, Indraneil Paul, Zhuang Li, Wen-Ding Li, Megan Risdal, Jia Li, Jian Zhu, Terry Yue Zhuo, Evgenii Zhettonozhskii, Nii Osae Dade, Wenhao Yu, Lucas Krauß, Naman Jain, Yixuan Su, Xuanli He, Manan Dey, Edoardo Abati, Yekun Chai, Niklas Muennighoff, Xiangru Tang, Muhtasham Oblokulov, Christopher Akiki, Marc Marone, Chenghao Mou, Mayank Mishra, Alex Gu, Binyuan Hui, Tri Dao, Armel Zebaze, Olivier Dehaene, Nicolas Patry, Canwen Xu, Julian McAuley, Han Hu, Torsten Scholak, Sébastien Paquet, Jennifer Robinson, Carolyn Jane Anderson, Nicolas Chapados, Mostofa Patwary, Nima Tajbakhsh, Yacine Jernite, Carlos Muñoz Ferrandis, Lingming Zhang, Sean Hughes, Thomas Wolf, Arjun Guha, Leandro von Werra, and Harm de Vries. StarCoder 2 and The Stack v2: The Next Generation, 2024. URL <https://arxiv.org/abs/2402.19173>.

Lannan Luo, Jiang Ming, Dinghao Wu, Peng Liu, and Sencun Zhu. Semantics-Based Obfuscation-Resilient Binary Code Similarity Comparison with Applications to Software Plagiarism Detection. In *Proceedings of the 22nd ACM SIGSOFT International Symposium on Foundations of Software Engineering, FSE 2014*, pp. 389–400, New York, NY, USA, 2014. Association for Computing Machinery. ISBN 9781450330565. doi: 10.1145/2635868.2635900. URL <https://doi.org/10.1145/2635868.2635900>.

Jean-Philippe Martin, Michael Hicks, Manuel Costa, Periklis Akrigidis, and Miguel Castro. Dynamically checking ownership policies in concurrent c/c++ programs. *SIGPLAN Not.*, 45(1):457–470, jan 2010. ISSN 0362-1340. doi: 10.1145/1707801.1706351. URL <https://doi.org/10.1145/1707801.1706351>.

Mayank Mishra, Matt Stallone, Gaoyuan Zhang, Yikang Shen, Aditya Prasad, Adriana Meza Soria, Michele Merler, Parameswaran Selvam, Saptha Surendran, Shivdeep Singh, Manish Sethi, Xuan-Hong Dang, Pengyuan Li, Kun-Lung Wu, Syed Zawad, Andrew Coleman, Matthew White, Mark Lewis, Raju Pavuluri, Yan Koyfman, Boris Lublinsky, Maximilien de Bayser, Ibrahim Abdelaziz, Kinjal Basu, Mayank Agarwal, Yi Zhou, Chris Johnson, Aanchal Goyal, Hima Patel, Yousaf

Shah, Petros Zerfos, Heiko Ludwig, Asim Munawar, Maxwell Crouse, Pavan Kapanipathi, Shweta Salaria, Bob Calio, Sophia Wen, Seetharami Seelam, Brian Belgodere, Carlos Fonseca, Amith Singhee, Nirmit Desai, David D. Cox, Ruchir Puri, and Rameswar Panda. Granite Code Models: A Family of Open Foundation Models for Code Intelligence, 2024. URL <https://arxiv.org/abs/2405.04324>.

Minh Huynh Nguyen, Nghi D. Q. Bui, Truong Son Hy, Long Tran-Thanh, and Tien N. Nguyen. HierarchyNet: Learning to Summarize Source Code with Heterogeneous Representations, 2023. URL <https://arxiv.org/abs/2205.15479>.

Erik Nijkamp, Bo Pang, Hiroaki Hayashi, Lifu Tu, Huan Wang, Yingbo Zhou, Silvio Savarese, and Caiming Xiong. A Conversational Paradigm for Program Synthesis. *arXiv preprint*, 2022.

OpenAI. GPT-4 Technical Report, 2023.

Kexin Pei, Zhou Xuan, Junfeng Yang, Suman Jana, and Baishakhi Ray. Trex: Learning execution semantics from micro-traces for binary similarity. *arXiv preprint arXiv:2012.08680*, 2020.

Kexin Pei, Jonas Guan, Matthew Broughton, Zhongtian Chen, Songchen Yao, David Williams-King, Vikas Ummadisetty, Junfeng Yang, Baishakhi Ray, and Suman Jana. StateFormer: Fine-grained type recovery from binaries using generative state modeling. In *Proceedings of the 29th ACM Joint Meeting on European Software Engineering Conference and Symposium on the Foundations of Software Engineering*, pp. 690–702, 2021.

Alec Radford and Karthik Narasimhan. Improving Language Understanding by Generative Pre-Training. 2018. URL <https://api.semanticscholar.org/CorpusID:49313245>.

Alec Radford, Jeff Wu, Rewon Child, David Luan, Dario Amodei, and Ilya Sutskever. Language Models are Unsupervised Multitask Learners. 2019.

Baptiste Rozière, Jonas Gehring, Fabian Gloeckle, Sten Sootla, Itai Gat, Xiaoqing Ellen Tan, Yossi Adi, Jingyu Liu, Tal Remez, Jérémie Rapin, Artyom Kozhevnikov, Ivan Evtimov, Joanna Bitton, Manish Bhatt, Cristian Canton Ferrer, Aaron Gratiafiori, Wenhan Xiong, Alexandre Défossez, Jade Copet, Faisal Azhar, Hugo Touvron, Louis Martin, Nicolas Usunier, Thomas Scialom, and Gabriel Synnaeve. Code Llama: Open Foundation Models for Code, 2023.

Andreas Sæbjørnsen, Jeremiah Willcock, Thomas Panas, Daniel Quinlan, and Zhendong Su. Detecting Code Clones in Binary Executables. In *Proceedings of the Eighteenth International Symposium on Software Testing and Analysis, ISSTA '09*, pp. 117–128, New York, NY, USA, 2009. Association for Computing Machinery. ISBN 9781605583389. doi: 10.1145/1572272.1572287. URL <https://doi.org/10.1145/1572272.1572287>.

Calif. Sausalito. Cybercrime Bytes: 10 Hot Security Certs, Public Safety Hacked, Intrusion's Shield. *Cybercrime Magazine*, 2020. URL <https://cybersecurityventures.com/cybercrime-bytes-10-hot-security-certs-public-safety-hacked-intrusions-shield/>.

Ensheng Shi, Yanlin Wang, Lun Du, Hongyu Zhang, Shi Han, Dongmei Zhang, and Hongbin Sun. CAST: Enhancing Code Summarization with Hierarchical Splitting and Reconstruction of Abstract Syntax Trees. In Marie-Francine Moens, Xuanjing Huang, Lucia Specia, and Scott Wen-tau Yih (eds.), *Proceedings of the 2021 Conference on Empirical Methods in Natural Language Processing*, pp. 4053–4062, Online and Punta Cana, Dominican Republic, November 2021. Association for Computational Linguistics. doi: 10.18653/v1/2021.emnlp-main.332. URL <https://aclanthology.org/2021.emnlp-main.332>.

Chad Spensky, Hongyi Hu, and Kevin Leach. LO-PHI: Low-Observable Physical Host Instrumentation for Malware Analysis. 2016.

Benjamin Steenhoek, Md Mahbubur Rahman, Richard Jiles, and Wei Le. An Empirical Study of Deep Learning Models for Vulnerability Detection. In *2023 IEEE/ACM 45th International Conference on Software Engineering (ICSE)*, pp. 2237–2248, 2023. doi: 10.1109/ICSE48619.2023.00188.

Zian Su, Xiangzhe Xu, Ziyang Huang, Zhuo Zhang, Yapeng Ye, Jianjun Huang, and Xiangyu Zhang. CodeArt: Better Code Models by Attention Regularization When Symbols Are Lacking, 2024.

Hanzhuo Tan, Qi Luo, Jing Li, and Yuqun Zhang. LLM4Decompile: Decompiling Binary Code with Large Language Models, 2024.

Hugo Touvron, Thibaut Lavril, Gautier Izacard, Xavier Martinet, Marie-Anne Lachaux, Timothée Lacroix, Baptiste Rozière, Naman Goyal, Eric Hambro, Faisal Azhar, Aurelien Rodriguez, Armand Joulin, Edouard Grave, and Guillaume Lample. LLaMA: Open and Efficient Foundation Language Models. *arXiv preprint arXiv:2302.13971*, 2023.

Laurens van der Maaten and Geoffrey Hinton. Visualizing Data using t-SNE. *Journal of Machine Learning Research*, 9(86):2579–2605, 2008. URL <http://jmlr.org/papers/v9/vandermaaten08a.html>.

Ashish Vaswani, Noam Shazeer, Niki Parmar, Jakob Uszkoreit, Llion Jones, Aidan N Gomez, Łukasz Kaiser, and Illia Polosukhin. Attention is All you Need. In I. Guyon, U. Von Luxburg, S. Bengio, H. Wallach, R. Fergus, S. Vishwanathan, and R. Garnett (eds.), *Advances in Neural Information Processing Systems*, volume 30. Curran Associates, Inc., 2017. URL https://proceedings.neurips.cc/paper_files/paper/2017/file/3f5ee243547dee91fdb053c1c4a845aa-Paper.pdf.

Hao Wang, Wenjie Qu, Gilad Katz, Wenyu Zhu, Zeyu Gao, Han Qiu, Jianwei Zhuge, and Chao Zhang. JTrans: Jump-Aware Transformer for Binary Code Similarity Detection. In *Proceedings of the 31st ACM SIGSOFT International Symposium on Software Testing and Analysis*, ISSTA 2022, pp. 1–13, New York, NY, USA, 2022. Association for Computing Machinery. ISBN 9781450393799. doi: 10.1145/3533767.3534367. URL <https://doi.org/10.1145/3533767.3534367>.

Yi Wu, Nan Jiang, Hung Viet Pham, Thibaud Lutellier, Jordan Davis, Lin Tan, Petr Babkin, and Sameena Shah. How Effective Are Neural Networks for Fixing Security Vulnerabilities. In *Proceedings of the 32nd ACM SIGSOFT International Symposium on Software Testing and Analysis*, ISSTA 2023, pp. 1282–1294, New York, NY, USA, 2023. Association for Computing Machinery. ISBN 9798400702211. doi: 10.1145/3597926.3598135. URL <https://doi.org/10.1145/3597926.3598135>.

Chunqiu Steven Xia, Yuxiang Wei, and Lingming Zhang. Automated Program Repair in the Era of Large Pre-Trained Language Models. In *Proceedings of the 45th International Conference on Software Engineering*, ICSE ’23, pp. 1482–1494. IEEE Press, 2023. ISBN 9781665457019. doi: 10.1109/ICSE48619.2023.00129. URL <https://doi.org/10.1109/ICSE48619.2023.00129>.

Guangxuan Xiao, Yuandong Tian, Beidi Chen, Song Han, and Mike Lewis. Efficient Streaming Language Models with Attention Sinks. In *The Twelfth International Conference on Learning Representations*, 2024. URL <https://openreview.net/forum?id=NG7sS51zVF>.

Xiangzhe Xu, Shiwei Feng, Yapeng Ye, Guangyu Shen, Zian Su, Siyuan Cheng, Guanhong Tao, Qingkai Shi, Zhuo Zhang, and Xiangyu Zhang. Improving Binary Code Similarity Transformer Models by Semantics-Driven Instruction Deemphasis. In *Proceedings of the 32nd ACM SIGSOFT International Symposium on Software Testing and Analysis*, ISSTA 2023, pp. 1106–1118, New York, NY, USA, 2023a. Association for Computing Machinery. ISBN 9798400702211. doi: 10.1145/3597926.3598121. URL <https://doi.org/10.1145/3597926.3598121>.

Xiangzhe Xu, Zhuo Zhang, Shiwei Feng, Yapeng Ye, Zian Su, Nan Jiang, Siyuan Cheng, Lin Tan, and Xiangyu Zhang. LmPa: Improving Decompilation by Synergy of Large Language Model and Program Analysis, 2023b.

Xiaojun Xu, Chang Liu, Qian Feng, Heng Yin, Le Song, and Dawn Song. Neural Network-based Graph Embedding for Cross-Platform Binary Code Similarity Detection. In *Proceedings of the 2017 ACM SIGSAC Conference on Computer and Communications Security*, CCS ’17, pp. 363–376, New York, NY, USA, 2017. Association for Computing Machinery. ISBN 9781450349468. doi: 10.1145/3133956.3134018. URL <https://doi.org/10.1145/3133956.3134018>.

Zhaoyan Xu, Antonio Nappa, Robert Baykov, Guangliang Yang, Juan Caballero, and Guofei Gu. AUTOPROBE: Towards Automatic Active Malicious Server Probing Using Dynamic Binary Analysis. In *Proceedings of the 2014 ACM SIGSAC Conference on Computer and Communications Security*, CCS ’14, pp. 179–190, New York, NY, USA, 2014. Association for Computing Machinery.

ISBN 9781450329576. doi: 10.1145/2660267.2660352. URL <https://doi.org/10.1145/2660267.2660352>.

Zichao Yang, Diyi Yang, Chris Dyer, Xiaodong He, Alex Smola, and Eduard Hovy. Hierarchical Attention Networks for Document Classification. In Kevin Knight, Ani Nenkova, and Owen Rambow (eds.), *Proceedings of the 2016 Conference of the North American Chapter of the Association for Computational Linguistics: Human Language Technologies*, pp. 1480–1489, San Diego, California, June 2016. Association for Computational Linguistics. doi: 10.18653/v1/N16-1174. URL <https://aclanthology.org/N16-1174>.

Wang Yue, Wang Weishi, Joty Shafiq, and C.H. Hoi Steven. CodeT5: Identifier-aware Unified Pre-trained Encoder-Decoder Models for Code Understanding and Generation. In *Proceedings of the 2021 Conference on Empirical Methods in Natural Language Processing, EMNLP 2021*, 2021.

Zhuo Zhang, Yapeng Ye, Wei You, Guanhong Tao, Wen-chuan Lee, Yonghui Kwon, Yousra Aafer, and Xiangyu Zhang. OSPREY: Recovery of Variable and Data Structure via Probabilistic Analysis for Stripped Binary. In *2021 IEEE Symposium on Security and Privacy (SP)*, pp. 813–832, 2021. doi: 10.1109/SP40001.2021.00051.

A APPENDIX

A.1 DATA COLLECTION

This section provides additional details of the data collection. To collect assemblies from The-Stack, we attempt to compile 4 million C programs, of which 138.8K is compiled successfully. We do not collect more due to the computation resource limitations.

For the 757.1K and 138.8K source code that successfully compiled into executables (using `gcc`) from AnghaBench and The-Stack, we disassemble them using `objdump`. `objdump` was not able to successfully disassemble all the executables, resulting in some empty assembly code. Thus, the number of 00 – 01 we obtain from each corpus is different and smaller than the number of source codes as shown in Table 1.

There may be alternative ways of collecting assembly code, e.g., using `gcc -S` to directly dump the assembly code without producing executables. However, a key difference is that the assembly generated by `gcc -S` does not undergo the linking step. In practice, binary decompilation and analysis are typically performed on executable or linked assembly code, as it includes linker modifications and reflects the final binary structure. Our data collection aligns better with the practical use of assembly. Nevertheless, Nova’s approaches should be generalizable to assembly code obtained with a different approach, and the experiments remain as future work.

Figure 6 shows an example of preprocessing the raw assembly code as described in Section 3.1.

<pre> 0: endbr64 4: push %rbp 5: mov %rsp,%rbp 8: mov %rdi,-0x8(%rbp) c: mov %rsi,-0x10(%rbp) 10: mov -0x8(%rbp),%rax 14: mov (%rax),%edx 16: mov -0x10(%rbp),%rax 1a: mov (%rax),%eax 1c: cmp %eax,%edx ... </pre>	<pre> : endbr64 : push rbp : mov rsp , rbp : mov rdi , -8 (rbp) : mov rsi , -16 (rbp) : mov -8 (rbp), rax : mov (rax), edx : mov -16 (rbp), rax : mov (rax), eax : cmp eax , edx : </pre>
(a) Raw Assembly	(b) Normalized Assembly

Figure 6: Example of assembly code preprocessing

A.2 EXPERIMENTAL SETUP DETAILS

This section provides additional details of training. We pre-train Nova starting from DeepSeek-Coder, using the language modeling objective (L_{lm}) for one epoch on the C functions and assembly functions collected from AnghaBench and The-Stack corpora. This step uses a batch size of 128, with the input

Table 10: Comparison with applying hierarchical attention on all attention heads, using 1B models.

Techniques	Pass@1					Pass@10				
	O0	O1	O2	O3	Avg.	O0	O1	O2	O3	Avg.
<i>Nova-HA</i>	30.58	19.88	20.58	16.40	21.86	44.75	33.13	33.31	29.82	35.25
Nova (hierarchical on all heads)	32.38	18.87	20.56	16.34	22.04	45.95	32.19	32.78	29.01	34.98
Nova	37.53	21.71	22.68	18.75	25.17	49.38	34.84	36.95	32.03	38.30

truncated by a 1,024 tokens limit. The model weights are updated using the AdamW optimizer. The learning rate is $5e^{-5}$, using 1000 steps of warm-up and a cosine decay to adjust the learning rate.

Then, the model is further pre-trained with the combination of language modeling and contrastive learning objectives ($L = L_{lm} + \lambda(L_{fcl} + L_{ocl})$), with λ set to 0.1. To train with the functionality contrastive learning objective, we discard any source code that misses any one of O0 – O3 assemblies and also discard the source code whose O2 assembly is the same as its O3 assembly. As a result, this step is only trained for 0.36M data samples for one epoch. The batch size is 64, with the input truncated by a 1,024 tokens limit. The learning rate is $2e^{-5}$ using the AdamW optimizer.

The fine-tuning of both BCD and BCSD uses a batch size of 64, with the input truncated by a 2,048 token limit. Similarly, the learning rate is $2e^{-5}$ using the AdamW optimizer, and the model is fine-tuned for one epoch. During the training using the contrastive learning objectives, and the fine-tuning of BCSD, we use the average of [INST] tokens’ last layer hidden states to represent the embedding of a binary function.

For the evaluation of BCSD, we reuse the framework provided by CodeArt Su et al. (2024) to evaluate the binary code similarity detection results once Nova produces the embeddings for functions in the test dataset. For each one of the K functions, the O0 assembly function is used as the query to calculate the cosine similarity between its embedding and the embeddings of all the K O3 assembly functions. Note that Nova does not normalize the embeddings of assembly functions during training and uses l_2 distance to calculate the L_{BCSD} , which optimize Nova to embed the O0 and O3 assembly functions from the same source code have the smallest l_2 distances. When using CodeArt’s framework for evaluation which ranks the similarity using the cosine similarity, we normalize Nova’s embedding for each assembly function since l_2 distance after normalization keeps the same order as cosine similarity (smaller l_2 distance means higher cosine similarity).

Infrastructure The experiments are conducted on eight NVIDIA RTX A100 GPUs, each with 40GB memory. Our implementation is based on Huggingface’s implementation of DeepSeek-Coder¹, PyTorch², and DeepSpeed³.

A.3 APPLYING HIERARCHICAL ATTENTION ON HALF ATTENTION HEADS

The hierarchical attention mask is always applied on half of the attention heads at each layer in Nova. This ensures the LLM balances the hierarchical knowledge of assembly code and pre-trained knowledge learned by full self-attention.

We conducted experiments applying hierarchical attention to all the attention heads. Results in Table 10 show that when applying hierarchical attention to all the attention heads of transformer layers, the performance does not improve enough and even drops under some settings. This implies that the standard full self-attention mechanism indeed learns knowledge that may not be captured by hierarchical attention. Thus, we only apply hierarchical attention to half of the attention heads in each transformer layer of Nova to balance the knowledge learned by standard and hierarchical attention.

A.4 ADDITIONAL ABLATION STUDY ON BINARY CODE DECOMPILE

We provide additional ablation studies on studying the impact of each individual contrastive learning objective. We study two more models:

- *Nova-FCL-HA*: Removing functional contrastive learning and hierarchical self-attention.

¹<https://huggingface.co/deepseek-ai/deepseek-coder-1.3b-base>

²<https://pytorch.org/get-started/locally/>

³<https://github.com/microsoft/DeepSpeed>

Table 11: Ablation study of Nova-1.3B on HumanEval-Decompile.

Techniques	Pass@1					Pass@10				
	O0	O1	O2	O3	Avg.	O0	O1	O2	O3	Avg.
Nova- <i>CL-HA</i>	20.73	16.16	15.03	11.19	15.78	33.55	28.12	26.96	21.01	27.41
Nova- <i>FCL-HA</i>	22.38	16.20	16.37	13.25	17.05	36.13	29.48	30.02	23.76	29.85
Nova- <i>OCL-HA</i>	28.44	18.87	18.53	15.76	20.40	40.28	32.33	31.80	27.05	32.87
Nova- <i>HA</i>	30.58	19.88	20.58	16.40	21.86	44.75	33.13	33.31	29.82	35.25
Nova	37.53	21.71	22.68	18.75	25.17	49.38	34.84	36.95	32.03	38.30

- Nova-*OCL-HA*: Removing optimization contrastive learning and hierarchical self-attention.

Table 11 shows that each component of the contrastive learning brings certain improvements to the Pass@1 and Pass@10 on HumanEval-Decompile, and we find the impact of function contrastive learning (FCL) is larger than the impact of optimization contrastive learning (OCL), suggesting that aligning the model’s embeddings for assembly code with the same functionality is more useful.

```
<func0>
0:  endbr64
4:  test   %esi, %esi
6:  jle    48 <func0+0x48>
8:  lea    -0x1(%rsi), %ecx
b:  add    $0x1, %rcx
f:  mov    $0x1, %edx
14: movss 0x0(%rip), %xmm3
1b: 00
1c: cmp    %rcx, %rdx
1f: je    4e <func0+0x4e>
21: movss -0x4(%rdi, %rdx, 4), %xmm2
27: mov    %rdx,%rax
2a: movaps %xmm2, %xmm1
2d: subss (%rdi, %rax, 4), %xmm1
32: andps %xmm3, %xmm1
35: comiss %xmm1, %xmm0
38: ja    54 <func0+0x54>
3a: add    $0x1, %rax
3e: cmp    %eax, %esi
40: jg    2a <func0+0x2a>
42: add    $0x1, %rdx
46: jmp    1c <func0+0x1c>
48: mov    $0x0, %eax
4d: retq
4e: mov    $0x0, %eax
53: retq
54: mov    $0x1, %eax
59: retq
```

O1 Assembly Code

```
int func0(float *arr, int n) {
    for (int i = 1; i < n; i++) {
        for (int j = 0; j < i; j++) {
            if (fabs(arr[i] - arr[j]) < 1.0f)
                return 1;
        }
    }
    return 0; GPT-4's Incorrect Decomilation
}
```

```
int func0(const float *x, int n) {
    int i;
    float diff = 1.0f;
    for (i = 1; i < n; i++) {
        if (fabs(x[i] - x[i-1]) > diff)
            return 0;
        return 1; LLM4Decompile's Incorrect Decomilation
    }
}
```

```
int func0(float *a, int n, float e) {
    int i, j;
    for (i = 0; i < n; i++)
        for (j = i + 1; j < n; j++)
            if (fabs(a[i] - a[j]) < e)
                return 1;
    return 0; Nova's Correct Decomilation
}
```

Figure 7: Nova-1.3B correctly decompiles HumanEval-Decompile task 0.

A.5 BINARY CODE DECOMPILE CASE STUDIES

Figure 7 shows an example from HumanEval-Decompile (task_id 0). Given the 01-optimized assembly code, GPT-4 fails to figure out the number of function arguments correctly, missing one important argument “float e”, and thus produces wrong functionality in the decompiled code. LLM4Decompile-1.3B makes similar mistakes and also misses the inner nested for loop. Nova-1.3B correctly decompiles the assembly into source code, where the ground truth is checking if any two elements in the given list *a* (with size *n*) are close to each other than a given threshold *e*.

Figure 8 shows another more complex example, HumanEval-Decompile task_id 20. Nova-1.3B correctly decompiles the source code, successfully figuring that the function is trying to find the two elements that are closest to each other in the given array *a*, with the result stored in *minmax*.

A.6 BINARY CODE SIMILARITY DETECTION ABLATION STUDY

Table 12, 13, 14, 15 show the detailed ablation study results of BCSD. Nova wins on the most benchmarks when *K* = 100 or 500, and ties with Nova-*HA* when *K* = 50, or 200.

```

<func0>:
0:    endbr64
4:    movss (%rdi), %xmm0
8:    movss %xmm0, (%rdx)
c:    movss 0x4(%rdi), %xmm1
11:   movss %xmm1, 0x4(%rdx)
16:   test %esi, %esi
18:   jle 8b <func0+0x8b>
1a:   lea  -0x1(%rsi), %r9d
1e:   mov $0x1, %r8d
24:   mov %rdi, %rcx
27:   movss 0x0(%rip), %xmm2
2e:   00
2f:   add $0x1, %r9
33:   movss 0x0(%rip), %xmm3
3a:   00
3b:   cmp %r8, %r9
3e:   je 82 <func0+0x82>
40:   mov %r8, %rax
43:   nopl 0x0%rax, %rax, 1
48:   movss (%rcx), %xmm1
4c:   movaps %xmm1, %xmm0
4f:   subss (%rdi), %rax, 4), %xmm0
54:   andps %xmm3, %xmm0
57:   comiss %xmm0, %xmm2
5a:   jbe 6d <func0+0x6d>
5c:   movss %xmm1, (%rdx)
60:   movss (%rdi), %rax, 4), %xmm1
65:   movaps %xmm0, %xmm2
68:   movss %xmm1, 0x4(%rdx)
6d:   add $0x1, %rax
71:   cmp %eax, %esi
73:   jg 48 <func0+0x48>
75:   add $0x1, %r8
79:   add $0x4, %rcx
...
99:   retq
O2 Assembly Code

```

```

void func0(float *a, int n, float *b) {
    int i, j;
    float min, max;

    min = max = a[0];
    for (i = 1; i < n; i++) {
        if (a[i] < min)
            min = a[i];
        else if (a[i] > max)
            max = a[i];
    }
    b[0] = min;
    b[1] = max; LLM4Decompile's Incorrect Decomilation
}

void func0(float *a, int n, float *minmax) {
    minmax[0] = a[0];
    minmax[1] = a[1];

    for (int i = 0; i < n; i++) {
        for (int j = i + 1; j < n; j++) {
            float diff = fabs(a[i] - a[j]);
            if (diff < minmax[1] - minmax[0])
            {
                minmax[0] = a[i];
                minmax[1] = a[j];
            }
        }
    }

    if (minmax[0] > minmax[1]) {
        float temp = minmax[0];
        minmax[0] = minmax[1];
        minmax[1] = temp;
    }
} Nova's Correct Decomilation

```

Figure 8: Nova-1.3B correctly decompiles HumanEval-Decompile task 20.

Table 12: Ablation study with $K = 50$.

Benchmarks	Nova- $CL-HA$	Nova- HA	Nova-1.3B
Binutils	0.86	<u>0.88</u>	0.87
Curl	0.84	0.87	<u>0.89</u>
ImageMagick	0.79	0.80	<u>0.86</u>
SQLite	0.80	<u>0.83</u>	0.77
OpenSSL	0.90	<u>0.92</u>	0.90
Putty	0.68	0.66	<u>0.72</u>
Avg.	0.81	0.83	<u>0.84</u>

Table 13: Ablation study with $K = 100$.

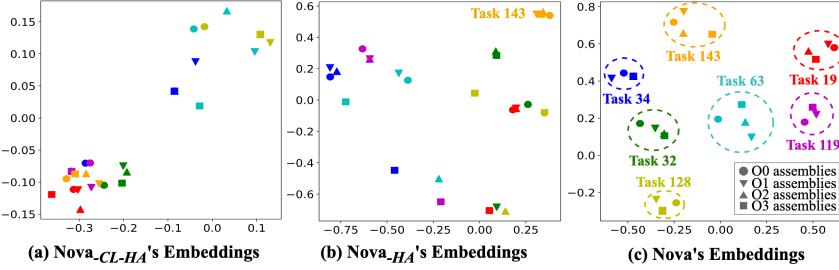
Benchmarks	Nova- $CL-HA$	Nova- HA	Nova-1.3B
Binutils	0.80	<u>0.82</u>	0.79
Curl	0.84	0.84	<u>0.86</u>
ImageMagick	0.70	0.72	<u>0.79</u>
SQLite	0.74	<u>0.78</u>	0.73
OpenSSL	<u>0.89</u>	<u>0.89</u>	0.88
Putty	0.59	0.60	<u>0.65</u>
Avg.	0.76	<u>0.78</u>	<u>0.78</u>

Table 14: Ablation study with $K = 200$.

Benchmarks	Nova- $CL-HA$	Nova- HA	Nova-1.3B
Binutils	0.71	<u>0.74</u>	0.73
Curl	0.80	0.73	<u>0.83</u>
ImageMagick	0.61	0.63	<u>0.73</u>
SQLite	0.68	<u>0.71</u>	0.68
OpenSSL	0.85	<u>0.87</u>	0.84
Putty	0.53	0.53	<u>0.55</u>
Avg.	0.70	0.70	<u>0.73</u>

Table 15: Ablation study with $K = 500$.

Benchmarks	Nova- $CL-HA$	Nova- HA	Nova-1.3B
Binutils	0.62	<u>0.65</u>	<u>0.65</u>
Curl	0.67	<u>0.71</u>	<u>0.73</u>
ImageMagick	0.46	0.51	<u>0.61</u>
SQLite	0.61	<u>0.62</u>	0.59
OpenSSL	0.77	<u>0.79</u>	0.78
Putty	0.46	0.46	<u>0.47</u>
Avg.	0.60	0.62	<u>0.64</u>

Figure 9: PCA of embeddings calculated by Nova-*CL-HA*, Nova-*HA*, and Nova.

A.7 ADDITIONAL ANALYSIS OF EMBEDDING

Figure 9 shows the results of PCA of embeddings provided by Nova-*CL-HA*, Nova-*HA*, and Nova, on randomly sampled seven examples, where Nova’s embeddings are consistently more distinguishable by functionalities.

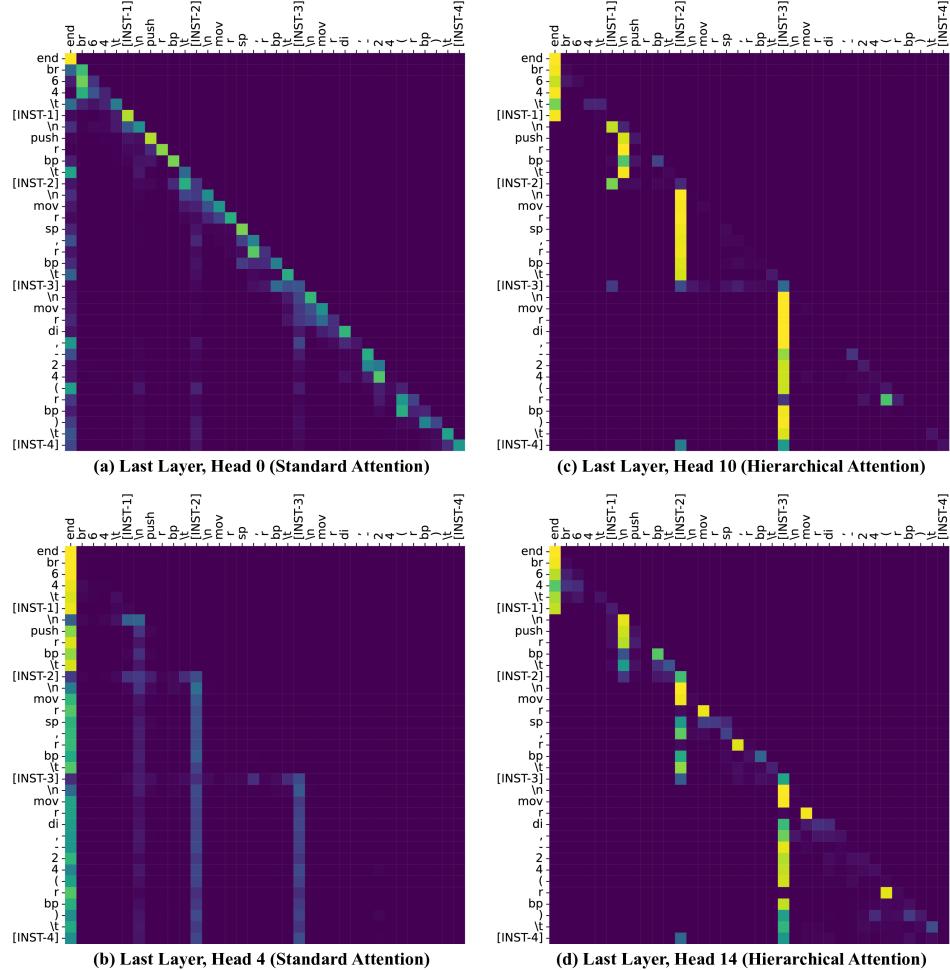


Figure 10: Comparison of attention distribution among standard and hierarchical heads.

A.8 ADDITIONAL ANALYSIS OF ATTENTION

Figure 10 shows the visualizations of attention weights in the final transformer layer of two select heads with standard attention and two heads with learned hierarchical attention. Standard attention

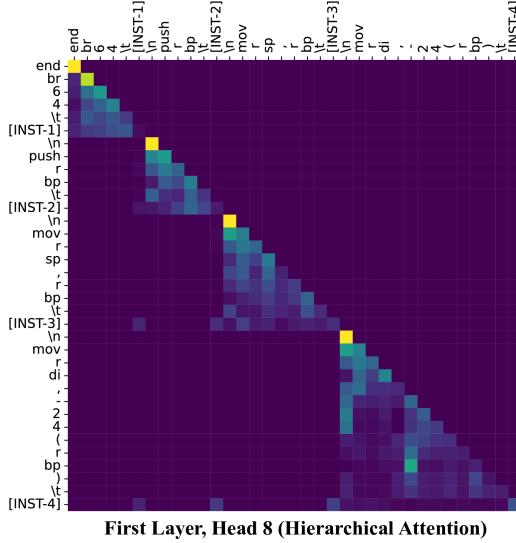


Figure 11: Learned per-instruction soft attention observed in the lower layers

exhibits two typical patterns, namely diagonal attention (i.e. tokens attending to themselves or nearby tokens, shown in Figure 10 (a)), and broad attention (i.e. a single token attending broadly to the entire sequence, shown in Figure 10 (b)). In contrast, in Nova’s hierarchical attention, attention weights are allocated among distinct segments, each corresponding to an instruction (shown in Figure 10 (c)), that focus on tokens comprising that instruction (e.g. opcodes and operands, shown in Figure 10 (d)), attentions are paid to “push”, “mov”, etc.).

Quantitatively, we have determined broad attention accounts for as much as 30% of all attention in standard heads, especially in layers 1-8 (consistent with the findings of (Clark et al., 2019)), whereas in Nova’s hierarchical attention, no more than 5% of all attention is allocated to each instruction segment. This validates our goal of learning instruction-aware hierarchical attention in Nova.

In addition, in lower layers, we have observed attention weights to be softly distributed among tokens comprising each instruction (Figure 11), which suggests Nova initially models cross-relations among operation codes and operands in the first few layers, and later pools their summary representation into the [INST] token in the later layers.

A.9 LIMITATIONS

One limitation is that Nova is X86-specific, as we only collect X86 assembly corpus for pre-training. This design choice is mainly affected by two facts: (1) X86 assembly is used and explored in a wide range of binary tasks (Wang et al., 2022; Su et al., 2024; Xu et al., 2023a; Chen et al., 2022c) compared to other assembly languages, and (2) computation limitations. However, the proposed techniques are independent of X86 assembly. Low information density and compiler optimization are the common challenges of most assembly languages such as X86, ARM, and MIPS. The proposed techniques can be applied to the future development of multi-lingual assembly LLMs. Another potential limitation is the scale of models. We develop Nova-1.3B and Nova-6.7B and demonstrate their advancement in assembly code decompilation and encoding. Developing larger Nova models is promising, but remains as future work due to limited computing resources.