# Can GPT-4 Perform Neural Architecture Search?

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## Abstract

*We investigate the potential of GPT-4 [36] to perform Neural Architecture Search (NAS)—the task of designing effective neural architectures. Our proposed approach, **GPT-4 Enhanced Neural archItectUre Search (GENIUS)**, leverages the generative capabilities of GPT-4 as a black-box optimiser to quickly navigate the architecture search space, pinpoint promising candidates, and iteratively refine these candidates to improve performance. We assess GENIUS across several benchmarks, comparing it with existing state-of-the-art NAS techniques to illustrate its effectiveness. Rather than targeting state-of-the-art performance, our objective is to highlight GPT-4's potential to assist research on a challenging technical problem through a simple prompting scheme that requires relatively limited domain expertise[1]. More broadly, we believe our preliminary results point to future research that harnesses general purpose language models for diverse optimisation tasks. We also highlight important limitations to our study, and note implications for AI safety.*

## 1. Introduction

Recent years have witnessed a string of high-profile scientific breakthroughs by applying deep neural networks to problems spanning domains such as protein folding [27], exoplanet detection [42] and drug discovery [44]. To date, however, successful applications of AI have been marked by the effective use of domain expertise to guide the design of the system, training data and development methodology.

The recent release of GPT-4 represents a milestone in the development of "general purpose" systems that exhibit a broad range of capabilities. While the full extent of these capabilities remains unknown, preliminary studies and simulated human examinations indicate that the model's knowledge spans many scientific domains [6, 36]. It is therefore of interest to consider the potential for GPT-4 to serve as a general-purpose research tool that substantially reduces the need for domain expertise prevalent in previous breakthroughs.

In this work, we investigate the feasibility of using GPT-4 without domain-specific fine-tuning to assist with a research task that has received considerable attention in the machine learning community: deep neural network design. Deep neural networks have proven effective on a diverse array of language and perception tasks, spanning domains such as question answering [39], object recognition [10, 29] and object detection [13, 32]. In the quest to improve performance, novel neural architecture designs, exemplified by proposals such as ResNets [15] and Transformers [52], have attained substantial gains in performance. Consequently, there has been significant interest in developing techniques that yield further improvements to neural network architectures. In particular, *Neural Architecture Search* (*NAS*) [62]—which seeks to automate the identification of optimal network configurations for specific tasks—has developed into an active area of research.

The starting point for this work was a pilot exploration that sought to assess whether GPT-4 possessed knowledge relevant for our target task, focusing specifically on the design of Convolution Neural Networks (CNNs). We began by simply prompting GPT-4[2]: ***"What are the design principles for a high-performance CNN model? Can you provide some examples based on your knowledge?"*** GPT-4 responded as follows: **(1) Depth**: Deeper networks can learn complex features and patterns. Increasing depth by adding more convolutional layers can improve performance while controlling overfitting. **(2) Width**: Increasing the number of filters in convolutional layers can help capture more diverse and complex features. Striking a balance between width and computational cost is crucial. **(3) Skip connec-

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[1]Code available at https://github.com/mingkai-zheng/GENIUS.

[2]*ChatGPT Mar 23 Version.*

**tions**: Skip connections allow gradients to flow through the network more easily, mitigating the vanishing gradient problem and enabling the training of deeper networks. **(4) Efficient computation**: Techniques like depthwise separable convolutions or group convolutions can reduce the number of parameters and computational costs without sacrificing performance. **(5) Normalization**: Normalization methods like batch normalization, layer normalization, or instance normalization can improve convergence and stability.

While the response to our rudimentary prompt lacks fine-grained specificity, it nevertheless suggests that GPT-4 possesses knowledge relevant to the target task. A natural next question then arises: does GPT-4 simply have "surface level" awareness of information related to this task, or does it have the depth of knowledge required to play a substantially greater role in the design and engineering of neural network architectures?

Our investigation seeks to address this question by examining the degree to which GPT-4 can propose effective neural network architecture designs. We view our work as a tentative exploration of the potential of GPT-4 to assist with scientific discovery, providing suggestions that enable rapid research prototyping on a challenging optimisation task. Further, we suggest that evidence of GPT-4's ability to search neural network architecture design spaces with limited input from human domain experts has implications for AI safety. However, we also emphasise the preliminary nature of our study and highlight some limitations (Sec. 5) to our methodology.

## 2. Related Work

### 2.1. Neural Architecture Design and Search

Neural architecture design plays a prominent role in deep learning research, with numerous studies focusing on developing architectural enhancements. Seminal works such as LeNet-5 [31], AlexNet [30], VGGNet [43], GoogleNet [49], ResNet [16], DenseNet [24], SENet [22] and Transformers [52] contributed design insights to improve performance. Numerous subsequent studies [20, 21, 24, 34, 41, 54, 59, 61] have further leveraged hand-crafted designs to explore the space of efficient, more capable architectures.

Neural Architecture Search (NAS) builds on many of these ideas but seeks a greater level of automation in the design process. Early efforts [62, 63] employed reinforcement learning to explore the search space of potential architectures, with later approaches leveraging evolutionary strategies [40] and Bayesian optimisation [28]. There has been considerable focus on reducing the computational burden associated with the search, with proposals such as DARTS [33] leveraging gradient-based search and EfficientNAS [37] employing sub-network sampling to increase efficiency. A rich body of work has further explored this direction [7, 9, 14, 26, 45, 47, 48, 50, 51, 57, 58, 58]. More recent work has employed evolutionary prompt engineering with soft prompt tuning to use language models for evolutionary NAS [8]. In contrast to conventional search strategies, we employ a process that simply prompts GPT-4 to propose designs from a given search space with a handful of examples.

### 2.2. Exploring GPT-4's research capabilities

Early studies in the technical report accompanying the release of GPT-4 [36] demonstrated that the model can achieve strong results across a broad suite of examinations designed to test human knowledge in widely-studied scientific disciplines such as biology, chemistry, physics, and computer science [2] etc.[3] A complementary set of preliminary qualitative studies conducted on an early variant of GPT-4 further highlight its ability to perform sophisticated reasoning across many topic areas [6], a further key building block for research applications. These studies also note important limitations in the model of relevance for research tasks - these include longstanding problems with "hallucinations" [35] and bias [4, 19], as well as an inability to construct appropriate plans in arithmetic and reasoning problems. Exploring applications in the chemistry domain, concurrent work explores how GPT-4 can be coupled to existing tools like web search and code execution to advance chemical research [1, 3]. Focusing on a different domain, we view our work as complementary to these explorations.

## 3. Approach

Our proposed method, GPT-4 Enhanced Neural Architecture Search (GENIUS), aims to tackle the challenging neural architecture search (NAS) problem by using GPT-4 as a "black box" optimiser. This entails first simply encoding the NAS problem statement into a human-readable text format that GPT-4 can parse. The model then responds with a model configuration proposal that aims to maximise a given performance objective (e.g., accuracy on a particular benchmark). GENIUS operates through an iterative refinement process. In the first iteration, we provide the problem encoding to the GPT-4 model which responds with an initial model configuration. Subsequently, we employ training and evaluation code to execute the model and obtain its empirical accuracy. This performance metric is then passed back to the GPT-4 model, prompting it to generate an improved model based on the insights gained from previous experiments. The algorithm is depicted in Algorithm 1.

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[3]We note that these results should be interpreted cautiously since the tests were designed for humans rather than language models. Nevertheless, they indicate some degree of familiarity with concepts that form prerequisites for various domains of scientific research.
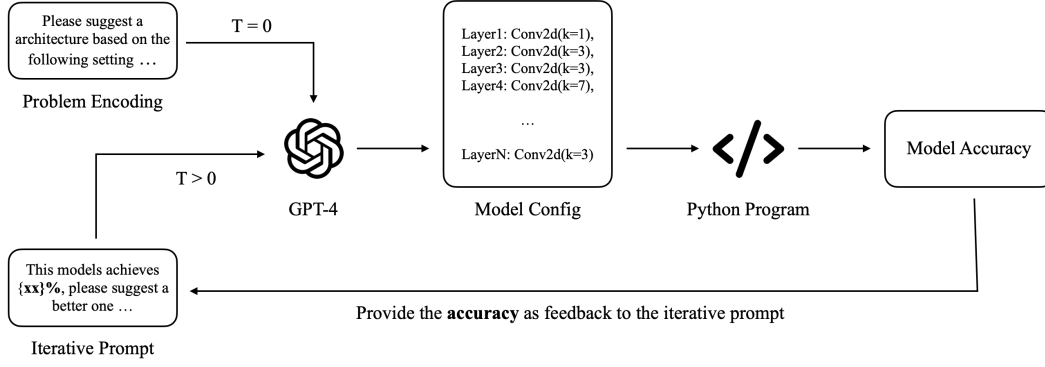
Figure 1. **An overview of the GENIUS framework**. After an initial problem encoding (corresponding to iteration $T = 0$), GPT-4 proposes a model configuration. A Python program is then executed to evaluate the quality of the configuration (assessed through its accuracy), and the results are passed back to GPT-4 via a natural language prompt for further iterations.

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**Algorithm 1:** GPT-4 Enhanced Neural Architecture Search (GENIUS)

**Input: GPT-4**: The GPT-4 API or ChatGPT Plus.
      **Problem_Encoding**: The human-readable text that encodes the NAS problem.
      **Run**: Function to train a given model configuration and return its accuracy.
      **T**: The number of iterations.

**for** *T=0 to iteration* **do**
  **if** *T == 0* **then**
    | model = GPT-4(Problem_Encoding)
  **else**
    prompt = "By using this model, we achieved an accuracy of {Accuracy}%. Please recommend a new model that outperforms prior architectures based on the above mentioned experiments. Also, Please provide a rationale explaining why the suggested model surpasses all previous architectures."
    model = GPT-4(prompt)
  **end**
  **Accuracy** = Run(model)
**end**
**Output:** The Best Model Configuration

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# 4. Proof of Concept

In this section, we first apply our GENIUS to two benchmark datasets to validate its effectiveness and empirically investigate its behavior. Following this, we assess the performance of the optimal architecture identified by GENIUS on the most widely-used benchmark in the NAS domain, comparing the results with other state-of-the-art methods.

## 4.1. Dataset and Benchmark

1. **NAS-Bench-Macro**[4] - This benchmark was first proposed in MCT-NAS [45] for single-path one-shot NAS methods. It consists of 6561 architectures and their isolated evaluation results on the CIFAR-10 dataset [29]. The search space of NAS-Bench-Macro is conducted with 8 searching layers, where each layer contains 3 candidate blocks. These blocks are marked as Identity, InvertedResidual Block with kernel size = 3 and expansion ratio = 3, and InvertedResidual Block with kernel size = 5 and expansion ratio = 6. Thus, the total size of the search space is $3^8 = 6561$.

2. **Channel-Bench-Macro**[5] - This benchmark was first proposed in BCNet [46] for channel number search. The search space of this benchmark is conducted with 7 searching layers, where each layer contains 4 uniformly distributed candidate widths. Thus, the overall search space is $4^7 = 16384$. It also provides the test results for all the 16384 architectures on CIFAR10 [29]. Additionally, this benchmark includes two base models, MobileNet [41] and ResNet [16].

## 4.2. Empirical Study

**Random Sampling Baseline.** In the realm of NAS, randomly sampled architectures are typically employed as a baseline. In the context of this study, we will utilize a stochastic function to uniformly sample from the available operations and channel numbers associated with each layer. Concretely, we will perform 10 sampling iterations and subsequently identify the most optimal architectures to serve as our baselines. Nevertheless, we observed considerable variance across individual trials resulting from this sampling approach. To address this, we repeated the 10-iteration pro-

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[4] https://github.com/xiusu/NAS-Bench-Macro
[5] https://github.com/xiusu/Channel-Bench-Macro

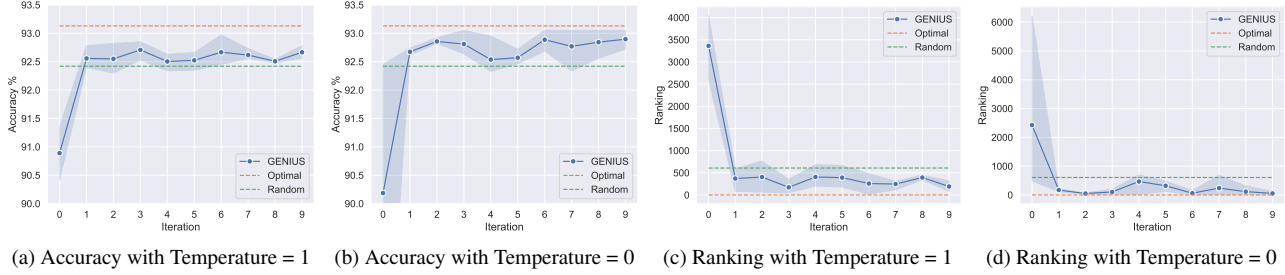| (a) Accuracy with Temperature = 1 | (b) Accuracy with Temperature = 0 | (c) Ranking with Temperature = 1 | (d) Ranking with Temperature = 0 |

Figure 2. We conduct experiments on **NAS-Bench-Macro** at two different temperatures: 0 and 1. Each experiment is repeated 3 times with 10 iterations per experiment. We show both the accuracy and ranking for each iteration. Note: higher accuracy and lower rankings correspond to better architectures.



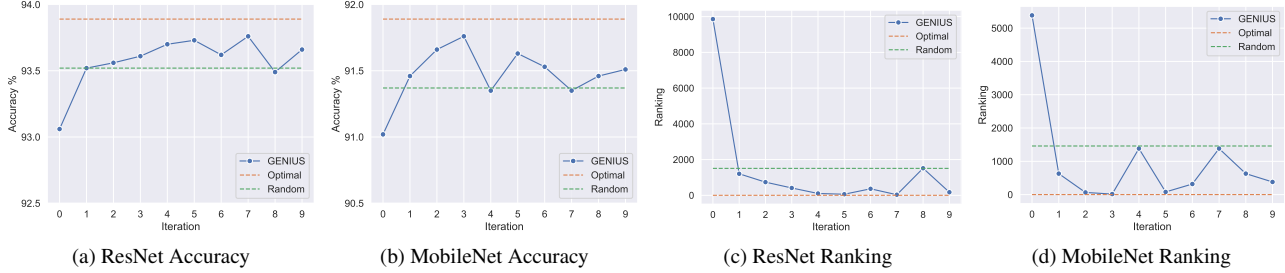| (a) ResNet Accuracy | (b) MobileNet Accuracy | (c) ResNet Ranking | (d) MobileNet Ranking |

Figure 3. We perform experiments on the **Channel-Bench-Macro** benchmark on both ResNet and MobileNet base models with a fixed Temperature of 0. Each experiment is conducted once for 10 iterations. We show both accuracy and ranking for each iteration. Higher accuracy and lower ranking correspond to a better architecture.

cess 10,000 times and calculated the average of the best outcomes.

**NAS-Bench-Macro**. To assess the effectiveness of GE-NIUS, we conduct an experiment using the NAS-Bench-Macro. For this experiment, we set the maximum number of iterations to 10. Since the benchmark provides ground truth accuracy values for each model configuration as a lookup table, we use these to retrieve the relevant accuracy score at each step. The GPT-4 API includes a *temperature* hyperparameter that controls the randomness of the model's output, with higher values leading to greater randomness in the output. We conducted experiments with both temperature=0 and temperature=1 to assess the effectiveness of GENIUS under different levels of randomness.

The experimental results are presented in Figure 2. We show both the accuracy and the model's ranking for each iteration. The best model obtained is ranked 8/6561 (Top 0.12%), while the worst model is ranked 61/6561 (Top 0.93%), remaining reasonable. (*We provide detailed numerical results for this experiment in Appendix A.3*) We observe that GENIUS exhibits some randomness in its responses, even when the temperature is set to 0. Nonetheless, despite this randomness, satisfactory results are achieved in the majority of cases.

**Channel-Bench-Macro.** We further evaluate the effectiveness of GENIUS on the Channel-Bench-Macro. In this experiment, we fix the temperature to 0 and perform only one trial on both ResNet and MobileNet settings. The experimental results are presented in Figure 3. Similar to the

previous experiment, we show the accuracy and rank for 10 iterations. Specifically, GENIUS achieves Rank 33 / 16384 (Top 0.2%) for the ResNet-based model and Rank 16 / 16384 (Top 0.1%) for the MobileNet-based model, further demonstrating its effectiveness. (*We provide detailed numerical results for this experiment in Appendix B.3*)

**Observations**. From the experiments, we can summarize the key observations regarding GENIUS's behavior:

1. Initial performance: At the first iteration, the accuracy and ranking of the generated models are relatively poor. This is expected, as GENIUS has not yet received any feedback to guide its architecture search.

2. Rapid improvement: In all trials, the accuracy improves quickly in the first few iterations, suggesting that GENIUS can effectively utilize the feedback from previous iterations to generate better models. The rank of the generated models also shows substantial improvement.

3. Stagnation: After a few iterations, the improvements in accuracy start to stagnate, with only minor fluctuations in accuracy and rank. This indicates that GENIUS may have reached a local optimum in the search space. Continuously requesting GENIUS to generate a better model forces it to produce a significantly different architecture from previous answers, which can lead to a much worse model before starting to converge again.

### 4.3. NAS-Bench-201

Next, we extend our application of GENIUS to the well-known NAS-Bench-201 [12] benchmark[6]. This benchmark focuses on designing a cell block for neural architectures. The cell in the search space is represented as a densely connected directed acyclic graph (DAG) consisting of four nodes and six edges, where nodes represent feature maps, and edges correspond to operations. With five available operations, the total number of possible search spaces amounts to $5^6 = 15625$. The performance will be evaluated on CIFAR10, CIFAR100, and ImageNet16-120.

Table 1. Experimental Results on NAS-Bench-201. We set **Temperature = 0** for GPT-4 in this experiment. We report the experimental results of all three trials for GENIUS. The underline indicates the second-best accuracy.

| Method | CIFAR10 | CIFAR100 | ImageNet16-120 |
|---|---|---|---|
| DARTS(1st) [33] | 54.30±0.00 | 15.61±0.00 | 16.32±0.00 |
| DARTS(2nd) [33] | 54.30±0.00 | 15.61±0.00 | 16.32±0.00 |
| SNAS [55] | 92.77±0.83 | 69.34±1.98 | 43.16±2.64 |
| PC-DARTS [56] | 93.41±0.30 | 67.48±0.89 | 41.31±0.22 |
| GDAS [11] | 93.61±0.09 | 70.70±0.30 | 41.71±0.98 |
| DSNAS [23] | 93.08±0.13 | 31.01±16.38 | 41.07±0.09 |
| iDARTS [60] | 93.58±0.32 | **70.83**±0.48 | 40.89±0.68 |
| **GENIUS (Ours)** | **93.84**±0.33 | 70.58±0.33 | **44.85**±0.57 |
| GENIUS (Trial 1) | 94.30 | 70.17 | 44.28 |
| GENIUS (Trial 2) | 93.64 | 70.60 | 45.63 |
| GENIUS (Trial 3) | 93.58 | 70.97 | 44.65 |

In accordance with previous experiments, we set the temperature parameter to 0 to minimize randomness and employ 10 iterations for GENIUS. Given that this benchmark provides both validation and test accuracy, we utilize validation accuracy for the prompt and report the test accuracy corresponding to the highest validation accuracy. Each experiment is conducted three times, with the results presented in Table 1. Notably, GENIUS surpasses other methods on the CIFAR10 and ImageNet16-120 datasets, achieving the highest accuracy scores of 93.84±0.33 and 44.85±0.57, respectively. On the CIFAR100 dataset, GENIUS attains the second-highest accuracy score of 70.58±0.33, marginally lower than the iDARTS method, which achieves 70.83±0.48. These experiments further substantiate the efficacy of GENIUS. (*We also provide the detailed numerical results along each iteration for this experiment in Appendix C.3*)

## 5. Limitations

We identify several important limitations to our study.

**Reproducibility.** First, we have little insight into the operations that wrap GPT-4 inference behind the API provided by OpenAI. For example, we do not know if our problem encoding text is pre-processed or if the model response is post-processed in some way (for example, by content moderation policies that are opaque to API clients). It is possible

that any such operations change over the course of an experiment, and we are unable to control for such changes. Second, even with the temperature set to 0, we observe some variation in GPT-4 responses, making it challenging to numerically reproduce a particular experimental run.

**Benchmark contamination.** We do not know which data was included in the training set for GPT-4, or the final cut-off date for training data provided to the model[7]. It is therefore possible that the benchmarks employed in our studies have all been "seen" by GPT-4, and thus it is searching "from memory" rather than leveraging insight about how to improve an architecture design. We note that previous studies examining the evidence of contamination have often found its effect on final performance to be somewhat limited [5, 38], perhaps due to the challenge of memorizing so much magnitude of the training data. Nevertheless, the fact that we cannot rule out contamination represents a significant caveat to our findings. One potential solution to address this in future work could be the construction of private optimisation benchmarks that are hidden from the open internet to ensure that they are excluded from the training data of large language models.

**Limited control and inscrutability.** Prompting represents our sole point of control over GPT-4, but we have relatively little understanding of how changes to the prompt influence behaviour as an optimiser. On the NAS-Bench-201 benchmark (see more details in Appendix C.3.), we find that later iterations under-perform earlier iterations in some cases, and it is unclear why this should be the case given that: (i) our prompt requests improved performance, (ii) our experimental evidence suggests that GPT-4 is capable of providing improved performance. We believe future work on this problem is particularly valuable.

## 6. AI safety

As AI systems become more capable, they exhibit greater potential for useful applications. However, they also represent greater risk—a concern that has been discussed by leading researchers within the field of AI for more than 60 years [53]. The use of GPT-4 as a black-box optimiser can potentially represent an offloading of intellectual labour from a human researcher to an inscrutable system. This contributes to the risk of *enfeeblement* [18] in which know-how erodes by delegating increasingly many important functions to machines. If general-purpose black-box optimisers ultimately prove superior to interpretable alternatives, competition pressures may incentivise such delegation [17]. Architecture search, in particular, represents a potential vector for self-improvement (potentially comple-

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[6]https://github.com/D-X-Y/NAS-Bench-201

[7]In [36], the authors note: *GPT-4 generally lacks knowledge of events that have occurred after the vast majority of its pre-training data cuts off in September 2021.... the pre-training and post-training data contain a small amount of more recent data.*

menting strategies that improve the inference capabilities of a trained model [25]). Such research can yield improved performance on tasks deemed beneficial by society, but may also exacerbate risk.

We believe it is useful to study whether existing, publicly available frontier models like GPT-4 possess such capabilities. Our tentative results (subject to the important limiting caveats described in Sec. 5), taken together with concurrent studies of scientific automation in other domains [1, 3], suggest that GPT-4 could potentially represent an artefact that leads to accelerated scientific research and therefore caution is appropriate in its application.

## 7. Conclusion

In this paper, we present GENIUS, a novel NAS approach that employs the GPT-4 language model as a black-box optimiser to expedite the process of discovering efficient neural architectures. We compare GENIUS against leading NAS methods, underscoring its effectiveness and highlighting the of GPT-4 as a tool for research and development. We also note safety implications and discuss several important limitations of our work. In future work, we plan to further study the capabilities and limitations of GPT-4 (and other frontier language models) to serve as optimisers in applications that have traditionally required extensive domain expertise, and to more extensively investigate the safety implications of such research.

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# A. Prompt for NAS-Bench-Macro

## A.1. System Prompt

You are an expert in the field of neural architecture search.

## A.2. User Prompt:

Your task is to assist me in selecting the best operations for a given model architecture, which includes some undefined layers and available operations. The model will be trained and tested on CIFAR10, and your objective will be to maximize the model's performance on CIFAR10.

We define the 3 available operations as the following:

```
0: Identity(in_channels, out_channels, stride)
1: InvertedResidual(in_channels, out_channels, stride expansion=3, kernel_size=3)
2: InvertedResidual(in_channels, out_channels, stride expansion=6, kernel_size=5)
```

The implementation of the Identity is as follows:

```
class Identity(nn.Module):
    def __init__(self, in_channels, out_channels, stride):
        super(Identity, self).__init__()
        if stride != 1 or in_channels != out_channels:
            self.downsample = nn.Sequential(
                nn.Conv2d(in_channels, out_channels, kernel_size=1, stride=stride, bias=False),
                nn.BatchNorm2d(out_channels),
            )
        else:
            self.downsample = None

    def forward(self, x):
        if self.downsample is not None:
            x = self.downsample(x)
        return x
```

The implementation of the InvertedResidual is as follows:

```
class InvertedResidual(nn.Module):
    def __init__(self, in_channels, out_channels, stride, expansion, kernel_size):
        super(InvertedResidual, self).__init__()
        hidden_dim = in_channels * expansion
        self.conv = nn.Sequential(
            nn.Conv2d(in_channels, hidden_dim, kernel_size=1, stride=1, padding=0, bias=False),
            nn.BatchNorm2d(hidden_dim),
            nn.ReLU(inplace=True),
            nn.Conv2d(hidden_dim, hidden_dim, kernel_size=kernel_size, stride=stride, padding=
    kernel_size//2, groups=hidden_dim, bias=False),
            nn.BatchNorm2d(hidden_dim),
            nn.ReLU(inplace=True),
            nn.Conv2d(hidden_dim, out_channels, 1, 1, 0, bias=False),
            nn.BatchNorm2d(out_channels),
        )
        self.use_shortcut = in_channels == out_channels and stride == 1

    def forward(self, x):
        if self.use_shortcut:
            return self.conv(x) + x
        return self.conv(x)
```

The model architecture will be defined as the following.

```
{
    layer1:  {defined: True,  operation: nn.Conv2d(in_channels=3,  out_channels=32, kernel_size=3,
    padding=1, bias=False)},
    layer2:  {defined: False, downsample: True , in_channels: 32,  out_channels: 64 , stride: 2},
    layer3:  {defined: False, downsample: False, in_channels: 64,  out_channels: 64 , stride: 1},
    layer4:  {defined: False, downsample: True , in_channels: 64,  out_channels: 128, stride: 2},
    layer5:  {defined: False, downsample: False, in_channels: 128, out_channels: 128, stride: 1},
```

```
7     layer6:  {defined: False, downsample: False, in_channels: 128, out_channels: 128, stride: 1},
8     layer7:  {defined: False, downsample: True , in_channels: 128, out_channels: 256, stride: 2},
9     layer8:  {defined: False, downsample: False, in_channels: 256, out_channels: 256, stride: 1},
10    layer9:  {defined: False, downsample: False, in_channels: 256, out_channels: 256, stride: 1},
11    layer10: {defined: True,  operation: nn.Conv2d(in_channels=256, out_channels=1280, kernel_size=1,
      bias=False, stride=1)},
12    layer11: {defined: True,  operation: nn.AdaptiveAvgPool2d(output_size=1)},
13    layer12: {defined: True,  operation: nn.Linear(in_features=1280, out_features=10)},
14  }
```

The currently undefined layers are layer2 - layer9, and the in_channels and out_channels have already been defined for each layer. To maximize the model's performance on CIFAR10, please provide me with your suggested operation for the undefined layers only.

Your response should be an operation ID list for the undefined layers. For example: [1, 2, ..., 0] means we use operation 1 for layer2, operation 2 for layer3, ..., operation 0 for layer9.

### A.3. Detailed Numerical Results for Figure 2

Table 2. Experimental Results on NAS-Bench-Macro. We set **Temperature = 1** for GPT-4 in this experiment. T is the iteration..

|         |         | T = 0 | T = 1 | T = 2 | T = 3 | T = 4 | T = 5 | T = 6 | T = 7 | T = 8 | T = 9 | Optimal |
|---------|---------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|---------|
| Trial 1 | Acc     | 90.90 | 92.40 | 92.30 | 92.53 | 92.63 | 92.66 | **92.97** | 92.56 | 92.50 | 92.56 | 93.13 |
|         | Ranking | 3440  | 590   | 766   | 353   | 203   | 180   | **19**    | 311   | 394   | 314   | 1 |
| Trial 2 | Acc     | 90.42 | 92.49 | 92.53 | **92.85** | 92.54 | 92.56 | 92.58 | 92.73 | 92.48 | 92.78 | 93.13 |
|         | Ranking | 4042  | 442   | 384   | **50**    | 332   | 331   | 272   | 119   | 446   | 82    | 1 |
| Trial 3 | Acc     | 91.35 | 92.78 | **92.82** | 92.74 | 92.34 | 92.35 | 92.45 | 92.56 | 92.54 | 92.66 | 93.13 |
|         | Ranking | 2609  | 83    | **65**    | 117   | 683   | 664   | 483   | 311   | 341   | 180   | 1 |

Table 3. Experimental Results on NAS-Bench-Macro. We set **Temperature = 0** for GPT-4 in this experiment. T is the iteration.. '-' denotes that GPT-4 asserts there is no chance to improve the performance further.

|         |         | T = 0 | T = 1 | T = 2 | T = 3 | T = 4 | T = 5 | T = 6 | T = 7 | T = 8 | T = 9 | Optimal |
|---------|---------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|---------|
| Trial 1 | Acc     | 85.70 | 92.62 | 92.82 | **93.05** | 92.95 | 92.46 | -     | -     | -     | -     | 93.13 |
|         | Ranking | 6221  | 212   | 64    | **8**     | 21    | 479   | -     | -     | -     | -     | 1 |
| Trial 2 | Acc     | 92.45 | 92.66 | **92.92** | 92.64 | 92.33 | 92.72 | -     | -     | -     | -     | 93.13 |
|         | Ranking | 496   | 189   | **27**    | 198   | 695   | 128   | -     | -     | -     | -     | 1 |
| Trial 3 | Acc     | 92.41 | 92.74 | **92.83** | 92.74 | 92.33 | 92.53 | 92.69 | 92.34 | 92.56 | 92.72 | 93.13 |
|         | Ranking | 564   | 113   | **61**    | 112   | 689   | 352   | 152   | 683   | 314   | 128   | 1 |

## B. Prompt for Channel-Bench-Macro

### B.1. System Prompt:

You are an expert in the field of neural architecture search.

### B.2. User Prompt:

Your task is to assist me in selecting the best channel numbers for a given model architecture. The model will be trained and tested on CIFAR10, and your objective will be to maximize the model's performance on CIFAR10.

The model architecture will be defined as the following.

```
1  {
2     layer1: nn.Conv2d(in_channels=3, out_channels=channels[0], kernel_size=3, padding=1, bias=False),
3     layer2: BottleneckResidualBlock(in_channels=channels[0], bottleneck_channels=channels[1],
       out_channels=channels[0], stride=1),
4     layer3: BottleneckResidualBlock(in_channels=channels[0], bottleneck_channels=channels[2],
       out_channels=channels[0], stride=1),
5     layer4: BottleneckResidualBlock(in_channels=channels[0], bottleneck_channels=channels[3],
       out_channels=channels[4], stride=2),
6     layer5: BottleneckResidualBlock(in_channels=channels[4], bottleneck_channels=channels[5],
       out_channels=channels[4], stride=1),
7     layer6: BottleneckResidualBlock(in_channels=channels[4], bottleneck_channels=channels[6],
       out_channels=channels[4], stride=1),
8     layer7: nn.AdaptiveAvgPool2d(output_size=1),
```

```
9        layer8: nn.Linear(in_features=channels[4], out_features=10),
10   }
```

The implementation of the BottleneckResidualBlock is as follows:

```
1   class BottleneckResidualBlock(nn.Module):
2       def __init__(self, in_channels, bottleneck_channels, out_channels, stride):
3           super().__init__()
4
5           self.stride = stride
6
7           self.block = nn.Sequential(
8               nn.Conv2d(in_channels, bottleneck_channels, 3, stride = stride, padding=1, bias=False),
9               nn.BatchNorm2d(bottleneck_channels),
10              nn.ReLU(inplace=True),
11              nn.Conv2d(bottleneck_channels, out_channels, 3, stride = 1, padding=1, bias=False),
12              nn.BatchNorm2d(out_channels),
13          )
14          self.relu = nn.ReLU(inplace=True)
15
16      def forward(self, x):
17          if self.stride == 1:
18              return self.relu(x + self.block(x))
19          else:
20              return self.relu(self.block(x))
```

For the 'channels' variable, the available channel number for each index would be:

```
1   {
2       channels[0]: [64, 128, 192, 256],
3       channels[1]: [64, 128, 192, 256],
4       channels[2]: [64, 128, 192, 256],
5       channels[3]: [128, 256, 384, 512],
6       channels[4]: [128, 256, 384, 512],
7       channels[5]: [128, 256, 384, 512],
8       channels[6]: [128, 256, 384, 512],
9   }
```

Your objective is to define the optimal number of channels for each layer based on the given options above to maximize the model's performance on CIFAR10. Your response should be the channel list consisting of 7 numbers (e.g. [64, 192, ..., 256]).

### B.3. Detailed Numerical Results for Figure 3

Table 4. Experimental Results on Channel-Bench-Macro with **ResNet**. We set **Temperature = 0** for GPT-4 in this experiment. T is the iteration.

|         | T = 0 | T = 1 | T = 2 | T = 3 | T = 4 | T = 5 | T = 6 | T = 7 | T = 8 | T = 9 | Optimal |
|---------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|---------|
| Acc     | 93.06 | 93.52 | 93.56 | 93.61 | 93.70 | 93.73 | 93.62 | **93.76** | 93.49 | 93.66 | 93.89 |
| Ranking | 9862  | 1205  | 737   | 411   | 103   | 61    | 365   | **33**    | 1515  | 173   | 1 |

Table 5. Experimental Results on Channel-Bench-Macro with **MobileNet**. We set **Temperature = 0** for GPT-4 in this experiment. T is the iteration.

|         | T = 0 | T = 1 | T = 2 | T = 3 | T = 4 | T = 5 | T = 6 | T = 7 | T = 8 | T = 9 | Optimal |
|---------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|---------|
| Acc     | 91.02 | 91.46 | 91.66 | **91.76** | 91.35 | 91.63 | 91.53 | 91.35 | 91.46 | 91.51 | 91.89 |
| Ranking | 5383  | 630   | 65    | **16**    | 1383  | 80    | 318   | 1383  | 630   | 380   | 1 |

## C. Prompt for NAS-Bench-201

### C.1. System Prompt:

You are Quoc V. Le, a computer scientist and artificial intelligence researcher who is widely regarded as one of the leading experts in deep learning and neural network architecture search. Your work in this area has focused on developing efficient algorithms for searching the space of possible neural network architectures, with the goal of finding architectures that perform well on a given task while minimizing the computational cost of training and inference.

## C.2. User Prompt:

You are an expert in the field of neural architecture search. Your task is to assist me in selecting the best operations to design a neural network block using the available operations. The objective is to maximize the model's performance.

The 5 available operations are as follows:

```
0: Zeroize()      # This operation outputs a tensor of zeros, effectively skipping the connection.
1: nn.Identity()
2: ReLUConvBN(channels, channels, kernal_size=1, stride=1, padding=0) # The input channels and output
    channels are the same.
3: ReLUConvBN(channels, channels, kernal_size=3, stride=1, padding=1) # The input channels and output
    channels are the same.
4: nn.AvgPool2d(kernel_size=3, stride=1, padding=1)                   # This operation does not change
    the spatial resolution.
```

The neural network block is defined by 6 operations (*i.e.*, op_list = [op0, op1, op2, op3, op4, op5]), which represent the operations executed between various stages of the block. This block comprises 4 stages, labeled as s0, s1, s2, and s3, each corresponding to distinct feature maps in the neural network.

s0 serves as the input feature map for this block.

s1 will be calculated by s1 = op0(s0).

s2 will be calculated by s2 = op1(s0) + op2(s1).

s3 will be calculated by s3 = op3(s0) + op4(s1) + op5(s2). Note that s3 becomes the output for this block and serves as the input for the subsequent block.

Then the implementation of the block will be:

```
class Block(nn.Module):
    def __init__(self, channels):
        super(Block, self).__init__()
        self.op0 = op_id_list[0]
        self.op1 = op_id_list[1]
        self.op2 = op_id_list[2]
        self.op3 = op_id_list[3]
        self.op4 = op_id_list[4]
        self.op5 = op_id_list[5]

    def forward(self, s0):
        s1 = self.op0(s0)
        s2 = self.op1(s0) + self.op2(s1)
        s3 = self.op3(s0) + self.op4(s1) + self.op5(s2)
        return s3
```

To construct our model, we intend to stack 15 of the Blocks that you have designed. Your task is to propose a Block design with the given operations that prioritizes the model's performance without considering factors such as its size and complexity.

## C.3. Detailed Numerical Results for NAS-Bench-201

Table 6. Experimental Results on NAS-Bench-201 with **CIFAR10**. We set Temperature = 0 for GPT-4 in this experiment. T is the iteration. We perform GENIUS on the validation set and report the final accuracy and ranking on the test set based on the best architectures verified on the validation set.

|  | T = 0 | T = 1 | T = 2 | T = 3 | T = 4 | T = 5 | T = 6 | T = 7 | T = 8 | T = 9 | Test Acc | Ranking |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Trial 1 (Validation) | 90.07 | 89.57 | 89.65 | 89.32 | **91.45** | 90.39 | 88.92 | 89.79 | 90.82 | 89.69 | 94.30 | 7 / 15625 |
| Trial 2 (Validation) | 90.54 | 89.53 | 89.83 | 90.17 | 89.71 | **90.82** | 89.94 | 88.81 | 90.47 | 90.15 | 93.64 | 280 / 15625 |
| Trial 3 (Validation) | **90.07** | 89.57 | 89.67 | 89.65 | 89.83 | 89.18 | 89.18 | 89.86 | 89.67 | 88.81 | 93.58 | 336 / 15625 |

Table 7. Experimental Results on NAS-Bench-201 with **CIFAR100**. We set Temperature = 0 for GPT-4 in this experiment. T is the iteration. We perform GENIUS on the validation set and report the final accuracy and ranking on the test set based on the best architectures verified on the validation set.

|  | T = 0 | T = 1 | T = 2 | T = 3 | T = 4 | T = 5 | T = 6 | T = 7 | T = 8 | T = 9 | Test Acc | Ranking |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Trial 1 (Validation) | 69.34 | 69.31 | 68.59 | 66.38 | 69.06 | **70.14** | 69.56 | 65.04 | 69.65 | 69.70 | 70.17 | 709 / 15625 |
| Trial 2 (Validation) | 69.47 | 68.31 | 68.85 | 63.01 | 68.35 | 68.45 | 66.74 | 66.75 | **70.54** | 68.49 | 70.60 | 394 / 15625 |
| Trial 3 (Validation) | **70.43** | 69.45 | 68.81 | 68.55 | 69.09 | 69.06 | 64.46 | 70.35 | 65.12 | 68.81 | 70.97 | 210 / 15625 |

Table 8. Experimental Results on NAS-Bench-201 with **ImageNet16-120**. We set Temperature = 0 for GPT-4 in this experiment. T is the iteration. We perform GENIUS on the validation set and report the final accuracy and ranking on the test set based on the best architectures verified on the validation set.

| | T = 0 | T = 1 | T = 2 | T = 3 | T = 4 | T = 5 | T = 6 | T = 7 | T = 8 | T = 9 | Test Acc | Ranking |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Trial 1 (Validation) | 44.19 | 40.47 | 37.31 | 36.58 | 39.96 | **44.43** | 43.52 | 37.48 | 40.30 | 42.92 | 44.28 | 636 / 15625 |
| Trial 2 (Validation) | **45.68** | 38.28 | 42.12 | 39.00 | 44.08 | 39.34 | 41.68 | 40.32 | 40.62 | 43.33 | 45.63 | 106 / 15625 |
| Trial 3 (Validation) | **45.75** | 43.15 | 44.68 | 41.90 | 41.78 | 44.62 | 41.11 | 44.23 | 41.51 | 38.38 | 44.65 | 434 / 15625 |