Function-constrained Program Synthesis

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Abstract

This work introduces: (1) a technique that allows pre-trained large language models (LLMs) to leverage user-provided code when solving programming tasks and (2) a method to iteratively generate modular sub-functions that can aid future code generation attempts when the initial code generated by the LLM is inadequate. Generating computer programs in general-purpose programming languages like Python poses a challenge for LLMs when restricted to using code provided in the prompt. A naive approach is to present a chat-based LLM (e.g. GPT-4) with relevant code snippets and prompt the model to synthesize the target algorithm using the provided code. Alternatively, code-specific LLMs (e.g. GitHub Copilot, CodeLlama2) can generate code completions in real-time by drawing on all code available in a development environment. However, restricting code-specific LLMs to use only in-context code is not straightforward, as the model is not explicitly instructed to use the user-generated code and users cannot highlight precisely which snippets of code the model should incorporate into its context for subsequent code-generations. Moreover, chat and code LLMs lack effective recovery methods, forcing users to iteratively re-prompt the model with modified prompts until a sufficient solution is reached.

Our method differs from traditional LLM-powered code-generation by constraining code-generation to an explicit function set and enabling recovery from failed attempts through automatically generated sub-functions. When the LLM cannot produce working code, we generate modular sub-functions to aid subsequent attempts at generating functional code. A by-product of our method is a library of reusable sub-functions that can solve related tasks, imitating a software team where efficiency scales with experience.

We also introduce a new "half-shot" evaluation paradigm that provides tighter estimates of LLMs' coding abilities compared to traditional zero-shot evaluation. Our proposed evaluation method encourages models to output solutions in a structured format, decreasing syntax errors that can be mistaken for poor coding ability.

1 Introduction

Given code-snippets, in the form of functions, and a high-level algorithm description (in natural language), we aim to generate a program, in a general-purpose language (Python), implementing the algorithm using the given functions and basic language operations, as displayed in Figure 1a. Doing so can enable automated integration of proprietary algorithms into existing infrastructure and can aid in bootstrapping development of new algorithms that build on existing code.

Recent advances in large language models (LLMs) show promising capabilities for code comprehension, correction, and generation [1, 2] but are still limited in their ability to implement complex and compositional programs [3]. A reason for this limitation is the LLMs' inability to iteratively implement and reuse functions in realtime when generating code. To make use of unseen (during training) functions without retraining a LLM, the functions must be provided within the model's

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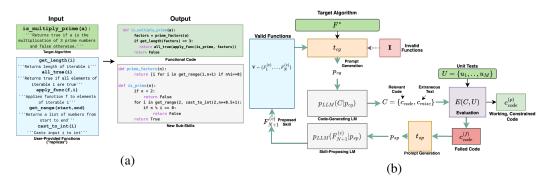


Figure 1: (a) Example input/output of our system on a question from HumanEval [8]. Custom replicas, handwritten versions of common Python functions, are used to implement the target algorithm. Subfunctions are produced as a by-product. (b) Method: we constrain a LLM to implement a target algorithm F^* using user-provided functions V and basic Python operations. When the model fails, we generate modular sub-functions $F_{N+1}^{(v)}$ to add to the function set, iteratively building a library until the constrained model can generate working code.

immediate context. Encouragingly, LLMs have demonstrated capabilities in using "tools", or API-calls, provided in-context [4, 5, 6, 7], which is analogous to generating calls to *functions* provided in-context. Motivated by this, we introduce here, to the best of our knowledge, the first methodology that not only primes LLMs to utilize in-context functions but also generates reusable sub-functions during program synthesis.

Designing a system that generates functional code while constrained to using user-specified functions presents several challenges. The main challenge is enabling the system to respond appropriately when it is initially unable to generate the desired algorithm. In particular, the system requires a robust failure handling mechanism that can break down complex programs into more tractable components. While simple techniques like resampling or feeding the error trace back into the model [9] as additional input may allow the system to eventually produce functional code, these approaches are inefficient and risk the system getting stuck on challenging tasks. Another challenge is ensuring the model can aptly use a user-provided function rather than reverting to behaviorally similar functions with which it is highly exposed to in training. A third challenge remains in ensuring that the output is presented in a usable format without requiring human postprocessing. Pre-trained LLMs are fine-tuned to produce outputs in specific, non-standard formats. If these formats are not anticipated, avoidable syntax errors can arise when evaluating the generated code [10].

Recent works have proposed various solutions aimed at addressing these challenges. Approaches leveraging classical program synthesis methods have introduced the concept of "library learning" [11, 12], exploring deductive algorithms which extract reusable components from an existing corpus of programs. While these works produce reusable function libraries as a byproduct of program synthesis, they often rely on domain-specific languages (DSLs) rather than general-purpose ones and require a heavy amount of input-output examples to specify the desired functions. LLMs such as GPT-4 [13] can generate code from more relaxed natural language specifications combined with a few input-output examples. More commonly, LLMs are often used as coding "assistants" that suggest and debug lines of code in an auto-regressive manner. These models (e.g. GitHub Copilot [14]) follow a limited range of context and produce code snippets in real-time to aid programmers. A coding-assistant, however, is designed to run alongside a human-programmer, and cannot be prompted to solve a number of problems on its own. Additionally, this approach does not currently allow the user to explicitly define which functions the LLM can and cannot use, making it difficult to ensure the model uses the desired functions. In a more autonomous fashion, "agents" (e.g., AutoGPT [15], BabyAGI [16], GPTEngineer [17], Aider [18]) can be initialized within a code-base and prompted to autonomously edit or generate code given the current context. Current agents, however, are not hard-coded with an effective way to handle cases when the model fails to produce working code and are prone to accumulation of compound hallucinations which can result in a loss of formatting structure and/or forgetting of the given functions.

Our approach addresses the aforementioned challenges as follows. We extend library learning to general-purpose languages and embed algorithm decomposition as an iterative process, allowing a greater margin of error per attempt than methods which rely on an initial "planning" step to decompose the entire problem (e.g. SelfPlanning [19]). To do this, we develop a prompting method to constrain a LLM to synthesise programs using only code (i.e., a set of functions) provided in-context, by the user. This allows the user to explicitly express which functions can and cannot be used in the generated code. If the constrained model fails to generate working code, we query an LLM to produce a new "sub-function" using only code provided in-context. The rationale is that the constrained model fails to generate working code because it lacks necessary functions in its context. We then add this sub-function to the set of valid functions to help the constrained model in future generation attempts - resulting in reusable functions as a byproduct - and iterate the process. A "half-shot" prompting and evaluation approach is introduced and used in all code-generation steps to ensure synthesize code is executable. We demonstrate the efficacy of our approach: achieving 73.1% accuracy on HumanEval [8] applying our method to GPT-3.5 [20] when constrained to an initial set of 21 hand-written functions designed to replicate behavior of common Python Standard Library (PSL) [21] functions. We also generate solutions for 17.4% questions in APPS [22] which were initially solved by the baseline GPT-3.5 but not solved by the constrained model even after 3 attempts.

2 Method

In Subsection 2.1, we outline three key steps of our method: (1) constraining a LLM to code provided in-context via prompting, (2) generating sub-functions to aid the next iteration of code-generation, and (3) incorporating sub-functions into LLM-generated code. In Subsection 2.2, we introduce the "half-shot" evaluation method. Examples for all prompts described are provided in supplementary material.

2.1 Key Steps

Constraining a LLM. We begin by constraining a LLM to a set of user-provided functions V and querying the constrained model to generate code. We model constrained code-generation as sampling code C from an LLM (formulated as a probabilistic function and what to expect upon return) conditioned on prompt p_{cg} , which is generated by "prompt-generator" (or prompt-template) t_{cg} (i.e. $C \sim p_{LLM}(C|p_{cg})$ where $p_{cg} = t_{cg}(F^*, V, I, p_f)$). Here, t_{cg} takes as its inputs the target algorithm F^* , formatting-instruction p_f , the set of valid functions V, and the set of invalid functions I as an input. The prompt generator t_{eq} is designed to maximize the likelihood that the constrained model will generate working code which (1) calls the user-provided functions and (2) does not call any functions outside of the valid set V. To encourage correct usage of a user-provided function, the prompt must include, at minimum, instructions for calling each function and input/output behaviour (since the model needs to know how to call the function), although providing a description of the function and/or full source code may be beneficial. In p_{cq} , we specify that only functions in V may be called in generated code. To further maximize the second objective, explicitly listing invalid functions I is useful when restricting use of functions highly exposed in LLM training (e.g. len(), all(); see Figure 1). In summary, the prompt p_{cq} is used to constrain the model and has the following high-level structure: a description of the target algorithm (e.g. a docstring), the set of valid user-provided functions (function names must be specified, but full code can also be provided), instructions to generate code utilizing only the valid user-provided functions (a set of invalid functions to explicitly restrict may also be specified), and formatting guidelines for the output code.

Generating Sub-functions. Code C sampled from the constrained LLM is evaluated for functional-correctness. Evaluation is formulated as a function E(C,U) which (1) parses relevant code c_{code} in C (removing any extraneous tokens, c_{misc}) and (2) evaluates c_{code} against unit-tests $U = \{u_1, ..., u_M\}$ (see Section 2.2 for more details). The code-evaluation block tags the code with a pass (p) or fail (f) and returns the tagged code as its output. When a constrained language model generates dysfunctional code (i.e. c_{code} fails a single unit-test) for a given task F^* , our approach requires generating a new sub-skill which, when added to the set of valid functions, $V = \{F_1^{(v)}, ..., F_N^{(v)}\}$, is intended to increase the probability of sampling working code from the constrained language model. We define sub-skills (i.e. sub-functions) as modular Python functions that may be useful in implementing the desired program F^* . A new sub-function, when added to the collection of valid functions in the

Table 1: Accuracy (pass@1) on HumanEval [8] with varying levels of formatting instruction provided in the prompt. Zero-shot prompt only includes the prompt provided by the dataset prompt (i.e. a docstring). The "basic" prompt adds "Complete the code." to the system prompt. The formatting-prompt/parser provides specific format instructions and parses outputs expecting that format. Both models perform drastically better when given stricter formatting instructions.

	Zero-shot	Basic	Formatting-string with parser (half-shot)
GPT-4	67.1%	73.7%	85.4%
GPT-3.5	34.1%	70.0%	71.3%

prompt, aims to enable the constrained model to generate working code in a subsequent attempt to implement the target algorithm. Sub-functions are proposed and implemented by sampling from a LLM conditioned on prompt p_{sp} : $F \sim p_{LLM}(F_{N+1}^v|p_{sp})$ where $p_{sp} = t_{sp}(c_{code}^{(f)}, F^*, V, I)$. Prompt p_{sp} follows the same high-level structure as prompt p_{cg} but instructs the model to generate a useful sub-function rather than code implementing the target algorithm. At minimum, the task description, F^* , valid functions V, and non-working code, $c_{code}^{(f)}$ are provided in prompt p_{sp} for context. We also consider the case where working, non-constrained (i.e. code which calls functions from I) code, f_{soln}^* , may be provided in-context in p_{sp} , serving as a reference to help predict a missing sub-function. In our experiments, f_{soln}^* is provided by the dataset or produced by an unconstrained language model.

Integrating Sub-Functions into LLM-Generated Code. To integrate a new sub-skill $F_{N+1}^{(v)}$ into subsequent code-generations we can simply add it to the set of valid functions V (i.e. $V \leftarrow \{F_{N+1}^{(v)}\} \cup V$; V is dynamically updated with the proposed sub-skill). This alone, however, is not sufficient. Because $F_{N+1}^{(v)}$ was implemented to aid specifically in solving algorithm F^* , it is likely that $F_{N+1}^{(v)}$ is more useful than other functions in the context of solving F^* , and should be distinguished within prompt p_{cg} , among $F^{(v)} \in V$. To do this, we introduce $V^* \subset V$ where V^* contains all $F^{(v)} \in V$ which have been specifically proposed to aid implementing the target algorithm F^* . We then formulate the new prompt with respect to this distinction: $p_{cg} = \hat{t}_{cg}(F^*, V^*, V, I, p_f)$. The updated prompt p_{cg} is used to condition the language model, from which a new solution to F^* is sampled. In our experiments, we only provide a single sub-function at-a-time ($|V^*| = 1$), although we investigate the effects of providing multiple sub-functions ($|V^*| > 1$) in an ablation included in supplementary material.

2.2 Half-Shot Evaluation

Typically, datasets like HumanEval [8] and APPS [22] provide a prompt describing the code to implement, which is fed directly to the code-generating model as the *only input* when evaluating for zero-shot performance. In this context "zero-shot" means that the only input to the model is the prompt provided by the dataset. The model's output is evaluated for functional correctness, generally through unit-testing. Pass@k accuracy [23] is reported. This evaluation methodology is problematic when models have inconsistent output formatting. Specifically, top-performing LLMs (e.g., GPT-4 [13], Claude-2 [24]) are often finetuned to behave interactively, generating conversational responses rather than completions. This causes variability in how outputs are formatted by default - some models tend to wrap code in markdown formatting like "triple backticks" or may include explanatory text before or after the code. These extraneous characters result in syntax errors when the output is evaluated, penalizing the model's score regardless of the functionality of the code provided [10].

In Table 1, pass@1 accuracy on HumanEval [8] with temperature set to 0 is reported using three prompt templates. Both GPT-4 and GPT-3.5 improve markedly when stricter formatting instructions are used, indicating *many zero-shot failures may be due to inaccurate formatting rather than coding inability.* For reference, the top performing model, Reflexion [25], achieves 91% accuracy on HumanEval. Other models, such as Parsel [26] (which achieves 85.1% accuracy), provide no additional performance beyond what a formatting-string and parser can provide.

To get a better, unbiased estimate of models' baseline coding-performance, we introduce a modified evaluation method focused on establishing upper bound estimates for a models coding-ability. Our

Table 2: "Half-shot" accuracy (pass@1) on HumanEval [8], $HE_{BP,R}$, and APPS [22] before and after constraining models' to only generate calls to functions (V_{rep}) provided in-context.

	HumanEval	${ m HE_{BP,R}}$	$APPS_{BP}$
GPT-4	85.4%	94.2%	-
GPT-4 Constrained	73.9%	78.2%	
GPT-3.5	71.3%	100%	100%
GPT-3.5 Constrained	65.8%	75.3%	10.4%

evaluation approach has three-steps: (1) Add a formatting-string to the prompt given by the dataset, instructing the model to formulate relevant code in as easy-to-parse format; (2) Parse the model output to extract the relevant code. The parser should strip non-code from model outputs before evaluation, minimizing syntax errors; (3) Evaluate the extracted code. In comparison to "zero-shot" evaluation, "half-shot" evaluation simply adds a formatting-string to the model input and passes the model's output through a parser. Although our evaluation method does not qualify as zero-shot, we maintain that no task-specific informational advantages are provided in-context in the evaluation step.

3 Experiments and Results

In this section, we first describe the datasets and sub-datasets used in our experiments. We then present the experiments leading to three key findings: (1) constraining a pre-trained LLM to unseen functions provided in-context degrades coding performance, (2) performance can be recovered by introducing appropriate sub-functions to the in-context function set, and (3) LLMs can automatically generate these useful sub-functions.

Datasets. Along with HumanEval (HE) [8] and APPS [22], four sub-datasets are relevant in our experiments: HE_{CF} contains 8 HumanEval questions which were answered correctly by the baseline GPT-3.5 model in a single attempt but failed when the model was constrained, even after three solutions were sampled at temperature (ϵ) set to 0.5; HE_{BFF} contains 19 HumanEval questions that neither the unconstrained baseline nor the constrained GPT-3.5 model could answer, even after three solutions were sampled with $\epsilon=0.5$; $HE_{BP,R}$ comprises 69 questions solved by the baseline unconstrained GPT-3.5 model (with $\epsilon=0$) that feature a free-standing function call in their solution (this set helps formulate V_{rep} described below) $APPS_{BP}$ contains 1329 questions from the APPS dataset which the unconstrained GPT-3.5 model successfully solved in a single attempt with $\epsilon=0$.

Constraining a LLM. We constrain both GPT-3.5 and GPT-4 to a set of functions denoted by V_{rep} which consists of 21 hand-written functions (e.g. get_length, all_true from Figure 1) designed to emulate the behavior of specific functions in the PSL, but under different names (e.g. len() becomes get_length()). This set of functions are referred to as "replicas," with each corresponding to an "origin function" in the PSL (details on all replicas is provided in supplementary material). The replicas are derived from all origin functions found in solutions to questions in $HE_{BP,R}$. Thus, constraining a model to using only replicas ensures no necessary functions are withheld when solving questions specifically in $HE_{BP,R}$. We constrain the models through prompting where prompts are constructed per-question from prompt generator t_{cg} as described in Section 2. We design t_{cg} (details provided in supplementary material) to maximize the Utilization Rate (UR; percent of solutions in which a function provided in-context is called) and minimize the Non-Compliance Rate (NCR; percent of solutions in which a function not provided in-context is called). Using the optimal t_{cg} , GPT-4 achieves a UR of 92.1% and NCR of 42.7% on HE [8]. The model utilizes the provided functions often, although it frequently invokes invalid functions as well. This is to be expected, since the original functions we replicated are among the most commonly used Python functions.

Having found an effective way to constrain GPT-3.5/4, we asses the functionality of the generated code. Table 2 provides the "half-shot" pass@1 accuracy of GPT-3.5 and GPT-4 with and without a constraint on various datasets. Importantly, we do not mark code incorrect specifically for using invalid functions. This allows us to independently evaluate change in the model's coding performance separately from its capacity to follow the constraint. On $HE_{BP,R}$, the accuracy of GPT-3.5 declines by 24.7% when constrained. This suggests that the constrained models' decrease in performance is not caused by restricting access to necessary functions, but rather from forcing the model to use

Table 3: GPT-3.5 constrained on replicas pass@1 accuracy after adding sub-skills to the set of usable functions provided in-context. We compare the efficacy of sub-skills generated by GPT-4, GPT-3.5 and a human expert, with and without (unconstrained) ground truth code f_{soln}^* provided for reference. Gain in parantheses refers to improvement above the baseline model (unconstrained GPT-3.5). Note that the baseline model failed all questions in HE_{CF} , HE_{BF} .

f_{soln}^*	Skill-Proposing LLM	HE	$\mathrm{HE}_{\mathrm{CF}}$	$\mathrm{HE}_{\mathrm{BFF}}$	$\mathrm{APPS_{BP}}$
Yes	Human Expert	-	100%	-	-
	GPT-4	-	62.5%	31.6%	-
	GPT-3.5	-	37.5%	15.8%	-
No	GPT-4	73.1%(+7.3)	50%	42.1%	-
	GPT-3.5	72.5% (+6.7)	62.5%	10.5%	17.6% (+7.2)

functions it has not seen in training. We analyzed all questions in $HE_{BP,R}$ which were passed by unconstrained GPT-3.5 but failed by constrained GPT-3.5 and found that none of the newly failed questions were a result of syntax errors (details provided in supplementary material). The decline in accuracy for the entire HumanEval dataset, -11.5% for GPT-4, is less marked than in $HE_{BP,R}$ because questions present in HumanEval but absent in $HE_{BP,R}$ are either already failed by the unconstrained baseline or solvable without the necessity of a replica. We attribute the 90% performance drop on the $APPS_{BP}$ dataset to the higher complexity of APPS questions compared to HumanEval. It is likely that the unconstrained model's baseline performance is inherently unstable for these questions. In summary, we find that GPT-3.5 and 4 perform worse on coding-tasks when they are instructed to generate code which can only contain calls to unseen functions provided in-context.

Providing Sub-Functions to the Constrained Models to Recover Performance. Here, we demonstrate that introducing sub-functions, as detailed in Section 2, can ameliorate some of the performance loss experienced after constraining the models. For each question in HE_{CF} we propose and handwrite a useful Python function which, when added to the set of functions provided in-context, increases the likelihood of drawing functional code from the constrained code-generating model when sampling a new solution to the previously failed question. As shown in the bottom row of Table 3, we are able to recover lost performance on 100% of questions in HE_{CF} by providing hand-written sub-functions. Note that the "human expert" meticulously crafted (through trial and error) the ideal sub-functions tailored for the HE_{CF} dataset to serve as an example of how performance can be fully restored given optimal sub-functions. Writing these functions by hand, however, is not scalable.

Generating Sub-Functions Automatically. Here, we demonstrate that sub-function generation can be scaled efficiently using LLMs. We employ GPT-3.5 and GPT-4 to independently propose and implement sub-functions intended help constrained models producing working code for questions in HumanEval [8], HE_{CF} , HE_{BFF} and $APPS_{BP}$. As in the previous experiment, each sub-skill is added to the set of functions provided in-context to GPT-3.5. Table 3 presents the "half-shot" pass@1 accuracy observed when sub-functions are provided. We consider the case when the skill-generating model is and is not provided ground-truth, unconstrained code f_{soln}^* . While LLM-generated subfunctions are not as effective as those generated by a human-expert (GPT-4's sub-functions result in +62.5% on HE_{CF}), LLM-generated sub-functions address challenges previously impassible by the constrained model alone. Impressively, providing automatically-generated sub-functions resolves nearly half of the questions that even the unconstrained model initially faltered upon (+42.1% on HE_{BFF}). The constrained GPT-3.5 model is also able to answer 73.1% of questions right on the HumanEval [8] dataset when GPT-4 produced sub-functions are provided in-context, surpassing the performance of the unconstrained GPT-3.5 model.

4 Conclusion

This report introduces a novel method for constrained program synthesis in a general purpose programming language using LLMs. Our experiments demonstrate that constraining LLMs like GPT-3.5 and GPT-4 to unseen functions provided in-context significantly reduces their ability to generate working code, with performance dropping by 11-89% across datasets. This highlights the limitations of LLMs when forced to use unfamiliar functions. To address this, we develop an iterative process to generate sub-functions that aid the model in solving tasks it previously failed on. Providing

sub-functions as this additional context enables the constrained models to recover much of the lost performance. Both GPT-3.5 and GPT-4 are able to automatically generate effective sub-functions that improve constrained model performance, increasing constrained GPT-3.5's accuracy on questions previously failed after 3 attempts by 62.5%.

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A Supplementary Material

We provide the following:

- In Section A.1, we present examples of prompts p_{cg} and p_{sp} used for code-generation and skill-proposals, respectively. We also provide examples of the prompts and parser used in motivating Half-Shot evaluation.
- In Section A.2, we present a list of all the replicas and their hand-written code.
- In Section A.3, we qualitatively compare outputs from GPT-3.5 before and after a constraint is applied.
- In Section A.4, we present a detailed report of all questions in $HE_{BP,R}$ failed by GPT-3.5 when constrained to the replicas.
- In Section A.5, we present details of an ablation on the size of V* briefly mentioned in the main paper.
- In Section A.6, we present a graphical overview of the sub-datasets used in our experiments.

A.1 Prompts

System Prompt

You are an intelligent programmer. You must complete the python function given to you by the user using only the functions they give you. And you must follow the format they present when giving your answer!

User Prompt

You have access to the following Python functions:

VALID FUNCTIONS {valid_functions}

The following functions may be particularly useful:

RELEVANT FUNCTIONS {relevant_functions}

You must complete the python function I give you using ONLY the given functions. You CANNOT use any of the following invalid functions:

INVALID FUNCTIONS {restriced_functions}

You must write the completion in the following form:

FUNCTION HEADER

START OF COMPLETION

• • •

You may only write your response in code/comments. Do not be verbose. The function you are to complete is:

{docstring}

Figure 2: Example code-generating prompt p_{cg} for an OpenAI chat model (GPT4/3.5). Constraints on valid and invalid functions are provided in the User Prompt. Alternatively, constraints can be specified in the Sytem Prompt. In our experiments, valid_functions (V) are the replicas (full code is provided), restricted_functions (I) is a list of the names of all the associated origin functions, and docstring (F*) describes the target algorithm. Particularly relevant_functions (V*) previously proposed in a function-generation step are distinguished. Using natural, commenting-style formatting instructions increases likelihood of correct formatting.

System Prompt

Follow the user instructions and provide an implementation of what you deem to be the most useful subfunction.

User Prompt

I have the following docstring: {docstring}

A correct completion to this function is: {unconst_comp}

I constrained a language model to generate a new completion using only custom Python functions that I provided. I gave it access to the following functions: {valid_functions}

It generated the following incorrect completion: {failed_completion}

Note that none of the following functions are allowed: {restricted_functions}

What new function would be useful to provide to the "constrained" language model to help it produce a working completion? Propose a completely new function. Only output code implementing the new function you propose. Only output executable code. Format your answer as follows:

BEGIN NEW-SUB FUNCTION ...

Figure 3: Example skill-proposal prompt for an OpenAI chat model (GPT4/3.5). This illustrates querying for a single sub-skill function, though the prompt could be modified to request multiple skills. In our experiments, valid_functions (V) are the replicas (full code is provided) and restricted_functions (I) is a list of the names of all the associated origin functions. The docstring (\mathbf{F}^*) and failed_completion ($c_{code}^{(f)}$) are included to provide context. Working code (f_{soln}^*) which does not adhere to the constraints is provided in this example.

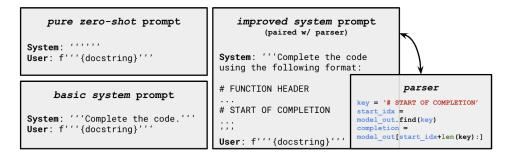


Figure 4: **Prompts used to Motivate Half-Shot Evaluation.** Basic zero-shot prompt (top left) only includes dataset prompt, i.e., docstring. Next level (bottom left) adds "Complete the code." to the system prompt. Final prompt (right) provides specific format instructions and parses outputs expecting that format.

A.2 Replicas

In this section, we provide details on the specific functions used to constrain the models in our experiments. The models are restricted to a particular set of functions, denoted by V_{rep} . A detailed overview of these functions can be found in Table 4.

Table 4: Hand-written code used for the Replicas. The corresponding function from the Python Standard Library is given in the left column.

Original function	Custom re-implementation (Replica)
	<pre>def get_length(iterable):</pre>
len()	<pre>count = 0 for _ in iterable:</pre>
	count += 1 return count
str()	<pre>def cast_to_string(input): return str(input)</pre>
chr()	def convert_to_char(input):
float()	return chr(input) def cast_to_float(input):
<u> </u>	return float(input) def cast_to_int(input):
int()	return int(input)
	<pre>def create_list(iterable=None): if iterable is None:</pre>
list()	return [] lst = []
	for item in iterable: lst.append(item) return lst
	<pre>def create_set(iterable=None): s = {}</pre>
set()	if iterable:
	for element in iterable: s[element] = None return s.keys()
	<pre>def check_if_instance(obj, class_or_tuple): if not isinstance(class_or_tuple, tuple):</pre>
isinstance()	class_or_tuple = (class_or_tuple,)
isinstance()	for cls in class_or_tuple: if type(obj) == cls or type(obj) in clssubclasses():
	return True return False
	<pre>def sort_list(iterable, key=None, reverse=False): lst = list(iterable)</pre>
	if key is None:
	compare = lambda a, b: a > b else:
sorted()	<pre>compare = lambda a, b: key(a) > key(b) for i in range(len(lst)):</pre>
	<pre>for j in range(len(lst) - 1): if compare(lst[j], lst[j + 1]):</pre>
	lst[j], lst[j + 1] = lst[j + 1], lst[j] if reverse:
	<pre>lst = lst[::-1] return lst</pre>
	<pre>def check_if_all_true(iterable):</pre>
all()	for element in iterable: if not element:
	return False return True
	<pre>def get_minimum(*args): if lor(orgs) == 1.</pre>
	<pre>if len(args) == 1: args = args[0]</pre>
min()	<pre>if not args: raise TypeError('expected at least 1 arguments, got 0')</pre>
()	min_val = args[0] for arg in args:
	<pre>if arg < min_val: min_val = arg</pre>
	return min_val
max()	def get_maximum(*args):
	return max_val def convert_to_binary(n):
	<pre>if n < 0: return '-' + convert_to_binary(-n)</pre>
bin()	result = '' while n:
·	result = ('1' if n & 1 else '0') + result
	<pre>n >>= 1 return '0b' + result if result else '0b0'</pre>
	<pre>def compute_sum(iterable, start=0): total = start</pre>
sum()	for item in iterable: total += item
	return total
	<pre>def round_number(number, ndigits=None): if ndigits is None:</pre>
round()	<pre>return int(number + 0.5) if number >= 0 else int(number - 0.5) else:</pre>
	factor = 10.0 ** ndigits
	return int(number $*$ factor $+$ 0.5 if number $>=$ 0 else number $*$ factor $-$ 0.5) $/$ factor

Table 4: Hand-written code used for the Replicas. The corresponding function from the Python Standard Library is given in the left column.

Original function	Custom re-implementation (Replica)	
math.ceil()	<pre>def get_ceiling(number): integer_part = int(number) if number == integer_part: return integer_part if number > 0: integer_part += 1 return integer_part</pre>	
math.sqrt()	<pre>def get_square_root(input, precision = 0.00001): guess = input / 2.0 while True: better_guess = (guess + input / guess) / 2.0 if abs(guess - better_guess) < precision: return better_guess guess = better_guess</pre>	
ord()	<pre>def get_unicode(char): if len(char) != 1: raise TypeError("Error." % len(char)) return int.from_bytes(char.encode('utf-8'), byteorder='big')</pre>	
map()	<pre>def apply_func_to_iterable(function, iterable): result = [] for item in iterable: result.append(function(item)) return result</pre>	
abs()	<pre>def absolute_value(number): if number < 0: return -number else: return number</pre>	
filter()	<pre>def add_to_list_if_func_is_true(function, iterable): result = [] for item in iterable: if function(item): result.append(item) return result</pre>	

 V_{rep} comprises 21 hand-written functions created to emulate common functions from the Python Standard Library. Hence, we call these functions "replicas." They are modeled on functions utilized by the unconstrained, baseline model during its evaluation on the HumanEval dataset. All replicas adhere to the following criteria:

- 1. A replica must maintain the same functionality as the original function it aims to imitate.
- 2. A replica must bear a distinct name from the corresponding original function, although the name should reflect its purpose. For instance, the replica mimicking len is named get_length.

In our experiments, we want to constrain the models to "replicas" in specific to ensure that we are not depriving the models of any essential resources they need to solve the problems in our dataset.

A.3 Examples of Model Output: Constrained vs. Unconstrained

```
Docstring

def cycpattern_check(a , b):
    ''''
    You are given 2 words. You need to return True if the second word or any of its rotations is a substring in the first word
    cycpattern_check("abcd","abd") => False
    cycpattern_check("hello","ell") => True
    cycpattern_check("whassup","psus") => False
    ''''
```

```
Unconstrained-Model Output

if len(a) < len(b):
    return False

if b in a:
    return True

for i in range(1, len(b)):
    if b[i:] + b[:i] in a:
        return True

return False</pre>
```

```
Constrained-Model Output
# Check if the length of b is
    greater than the length
   of a
if get_length(b)>get_length(a
   ):
    return False
# Concatenate a with itself
   to check for rotations of
a = a + a
 Check if b is a substring
   of a or any of its
   rotations
if b in a:
    return True
return False
```

Figure 5: Comparing Outputs from Constrained and Unconstrained GPT-3.5. This figure shows the responses of GPT-3.5, in both constrained and unconstrained conditions, to a particular question involving the detection of cyclic patterns within strings. On the left, the Unconstrained-Model adheres to logic and a succinct approach. On the right, the Constrained-Model commits logical errors, beginning with the unnecessary concatenation of string a with itself. This discrepancy highlights the decrease in performance that may arise when a model is constrained to use replicas of common functions. The upper part of the figure shows the docstring, which outlines the specifications of the cycpattern_check function.

A.4 Analyzing Failure Cases on $HE_{\mathrm{BP},\mathrm{R}}$

Table 5: Detailed report of failures when prompted to use custom sub-functions.

Task ID	Desc. of Failure	Failure Categorization
144	casts a string fraction to a float instead of splitting numerator and denominator first	logic
65	does not reverse string if shift % length = 0 (should always reverse when shift > len)	logic
124	assumes string formatting is correct (can be split on the '-'); does not account for leap years	logic
149	sorts by string value rather than string length and alphabetically	logic
114	restarts sub-array if element is negative rather than if it is less than current element	logic
79	does not remove the 0b prefix from the convert_to_binary func.	logic (didn't understand custom func well)
142	does not include the case where index is not 3 or 4	logic
121	selects odd position elements instead of even by starting at index 1 instead of 0	logic
89	does not mod by 26 to ensure staying within alphabet	logic
97	needs to separate modulo operations by a parentheses	logic
154	does not correctly check rotations of b	logic
99	always rounds negative numbers toward 0, even when decimal part is greater than or equal to -0.5	logic
110	returns "yes" prematurely after checking if lst2 has even elements	logic
84	converts char to bin then bin to int instead of char to int	logic
70	does not recompute min and max value within the while loop	logic
82	used get_ceiling() when floor should've been used	logic
90	does not account for multiple smallest elements (i.e. [1,1] case) originally avoided by converting list to a set	logic

A.5 Determining the Optimal Number of Sub-Functions to Provide, Per Question

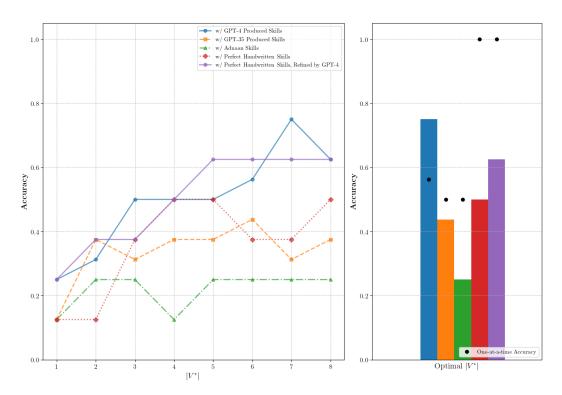


Figure 6: Impact of $|V^*|$ on Performance in HE_{CF} . This figure analyzes the relationship between the number of functions included in V^* and performance on the HE_{CF} dataset, using functions proposed by GPT-4 (blue), GPT-3.5 (orange), and a human expert (red). The batch of functions marked in purple are the perfect-handwritten skills after being refined by GPT-4. Results for sub-skills proposed by a non-expert human (Adnaan) are presented in green. The black dot on the right bar plot represents the naive expected accuracy when the optimal number of sub-skills are included, which should (naively) match the average accuracy across all 8 questions when only a single function is included in the constrained model's context when solving the related question. The model is only able to achieve 50% of its one-at-a-time accuracy when all human-written functions are provided (red bar plot). But when providing all functions generated by GPT-4 the model outperforms its one-at-a-time accuracy (blue bar plot).

In our experiments, for a given question only the sub-function generated with respect to the question is provided to the constrained model on its subsequent attempt at solving the given question (i.e. $|V^*|=1$). Here, we explore how varying the number of functions in V^* influences model performance. We consider four-sets of 8 functions generated for each HE_{CF} question by GPT-4, GPT-3.5, a non-expert human (Adnaan), and a human-expert. In each set (e.g., GPT-4's proposed set) of 8 proposed subfunctions, each sub-function is proposed with the intention of supporting only one unique problem in HE_{CF} . For each set of 8 proposed functions, we vary the inclusion of these functions (from 1 to 8) within V^* and evaluate replica-constrained GPT-3.5 performance on all questions in HE_{CF} . When a sub-function is ablated from V^* , it is also made absent from V, meaning that the model is not provided the sub-function in any way. Performance is compared against the average accuracy across all 8 questions obtained when providing a sub-function solely to its corresponding HE_{CF} question. We call this the 'one-at-a-time-accuracy'. The naive assumption is that when all functions are integrated into V^* , the accuracy should mirror the average 'one-at-a-time' configuration.

Our results, presented in Figure 6 show that this is not the case. We find that when the optimal amount of functions included (i.e., the $|V^*|$ which maximises accuracy), there is variability in how the model performs in comparison to the expected one-at-a-time accuracy. For example, when using the "perfect" set of handwritten functions (deemed perfect because when the functions are fed one-at-a-time to their intended question, all questions pass) the model only achieves 50% of

its one-at-a-time accuracy when all functions are provided (red bar plot). But when providing all functions generated by GPT-4, the model achieves 120% of its one-at-a-time accuracy (blue bar). In general, we see that GPT-generated functions, when provided to a constrained model alongside other functions, result in better performance than when handwritten functions are fed alongside other functions. Due to the small sample size of questions (8), this can be attributed to the stochastic nature of GPT-3.5 (i.e., arbitrary variations in the prompt produce better/worse performance). However, if this is not the case, then this implies that the GPT models are formulating functions in a way that, when fed among a batch of other functions, allows the LM to better use the right function for the right problem.

To test this hypothesis, we took all functions in the set of expert-written functions (red) and asked GPT-4 to "Make this function more understandable." We then evaluated the results of this new set of refined functions, shown in purple. Although the refined set results in better performance than the non-refined set, the refined set only achieves 62% of its one-at-a-time accuracy. This results indicates that the functions in the handwritten set overfit the one-at-a-time scenario where they are the only sub-function being provided to the model. This means that they are perfectly crafted to trigger the model to output the correct solution when fed alone, but when combined with other functions (i.e., a variation in the prompt) the correct response isn't generated, implying that the human-written functions do not generalise as well as GPT-generated functions to scenarios where multiple functions are provided at once.

A.6 Sub-Datasets

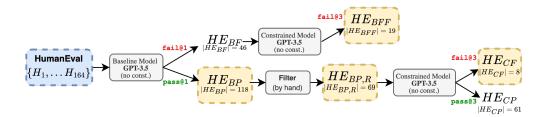


Figure 7: **Sub-datasets extracted from HumanEval.** Relevant sub-datasets are highlighted in yellow. HE_{BFF} includes the questions that the original, unconstrained model failed to solve with just one attempt. On the other hand, HE_{CF} comprises questions that the baseline, unconstrained model answered correctly, but the constrained model could not solve. Both of these sub-datasets undergo a refinement process, where the constrained baseline model is allowed three more attempts at answering all questions (with temp = 0.5). This step ensures that any future successes in our experiments are more likely a result of genuine improvement rather than random chance.

Four sub-datasets are extracted from HumanEval and used in our experiments. One sub-dataset, $APPS_{BP}$, is extracted from APPS. Refer to Fig. 7 for a visual guide explaining the extraction of the HumanEval sub-datasets.

 $\mathbf{HE_{BP}}$. The first sub-dataset, HE_{BP} , consists of 118 questions. These questions are sourced from those that the baseline model, GPT-3.5, can answer in one attempt using the "half-shot" pass@1 method, without any constraints. The aim of HE_{BP} is to pinpoint questions correctly addressed by the original unconstrained model.

 $\mathbf{HE_{BP,R}}$. The second sub-dataset, $HE_{BP,R}$, comprises 69 questions. These are extracted from HE_{BP} by manually identifying questions whose answers contain at least one free-standing function call, such as len(.) or math.sqrt(.). The function calls identified serve as a reference to construct V_{rep} , as detailed in Table 4. The primary goal of $HE_{BP,R}$ is to spot questions from the unconstrained model that feature a free-standing function call in their solutions. This set helps formulate V_{rep} .

 $\mathbf{HE_{CF}}$. The third sub-dataset, HE_{CF} , encompasses 8 questions. These are derived by testing the baseline GPT-3.5, but this time constrained on V_{rep} , on $HE_{BP,R}$ with a three-attempt limit, and collecting all the unanswered queries. HE_{CF} is designed to ensure that if our method improves a model's performance on a question from this set during tests, it is likely due to our specific improvements and not mere randomness. This dataset aids in gauging the effectiveness of introducing sub-functions.

 $\mathbf{HE_{BFF}}$. The fourth sub-dataset, HE_{BFF} , has 19 questions, obtained in a two-step manner:

- 1. Initially, we gather questions the baseline model, GPT-3.5, fails to answer in one attempt using the "half-shot" pass@1 method, without constraints.
- 2. Following that, we test the constrained GPT-3.5 on V_{rep} on the previously collected questions, allowing for three tries, and select all the incorrectly answered ones.

The purpose of HE_{BFF} is to represent the questions that the original, unconstrained model couldn't solve in one attempt (as described in step 1). In our experiments, we want to decrease the likelihood that the questions in this dataset are passed just by random chance, rather than because of the improvements introduced by our method. To do this, we use the process in step 2 to refine and confirm the questions that were selected from step 1.

APPS_{BP}. $APPS_{BP}$ consists of 1329 questions from the APPS dataset which the unconstrained GPT-3.5 does not pass with one attempt (i.e., using "half-shot" pass@1). This sub-dataset is similar to HE_{BP} , but derived from APPS rather than HumanEval.