iPrompt: Explaining Data Patterns in Natural Language via Interpretable Autoprompting

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Abstract

Large language models (LLMs) have displayed an impressive ability to harness natural language to perform complex tasks. We explore whether we can leverage this ability to find and explain patterns in data. Specifically, given a pre-trained LLM and data examples, we introduce interpretable autoprompting (*iPrompt*), an algorithm that generates a natural language string explaining the data. iPrompt iteratively generates explanations with an LLM and reranks them based on their performance when used as a prompt. Experiments on a wide range of datasets, from synthetic mathematics to natural language understanding, show that iPrompt can yield meaningful insights by accurately finding dataset explanations that are human-interpretable. On two of four classification datasets, iPrompt discovers a prompt that outperforms human-written prompts on GPT-3, despite only querying the relatively small GPT-J model. Finally, experiments with scientific datasets show the potential for iPrompt to aid in scientific discovery. [1]

1. Introduction

Large language models (LLMs) have attained an extraordinary ability to harness natural language for solving diverse problems (Devlin et al., 2018), often without the need for finetuning (Brown et al., 2020; Sanh et al., 2021). Moreover, LLMs have demonstrated the capacity to excel at real-world problems, such as mathematics (Lewkowycz et al., 2022), scientific question answering (Sadat & Caragea, 2022), general processing of scientific text (Beltagy et al., 2019), predicting brain responses (Schrimpf et al., 2021), and classifying proteins and chemical compounds (Taylor et al., 2022).

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[1]All code for using the methods and data here is made available on Github.
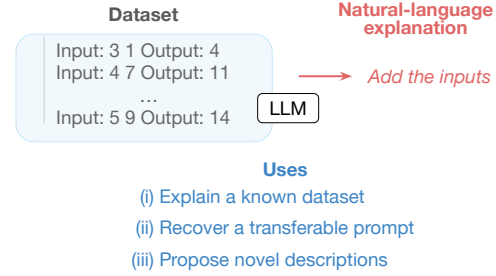

Figure 1. Interpretable autoprompting (*iPrompt*) inverts the standard prediction problem to instead find a natural language explanation of the data using a fixed, pre-trained large language model.

In this work, we probe whether we can leverage the learned skills of an LLM to *discover and explain patterns* in a dataset. To do so, we invert the typical problem of fitting an LLM to data and instead ask whether we can use a fixed LLM to produce a natural language string explaining dataset patterns.

Our approach to this problem centers around prompting. Prompting has emerged as an effective method for adapting LLMs to new datasets (Liu et al., 2021a); a prompt string is combined with each example in a dataset before querying an LLM for an answer. While prompts were initially constructed manually, recent work has shown success in *autoprompting*, automatically finding a prompt via optimization (Shin et al., 2020; Li & Liang, 2021; Deng et al., 2022). However, previous work on learning natural language prompts does not produce prompts that are meaningful to humans.

Our approach, interpretable autoprompting (*iPrompt*), extends autoprompting to generate a semantically meaningful natural language prompt that explains a key characteristic of the data (see Fig. 1). For example, given a dataset of examples of addition, e.g. 2 5 ⇒ 7 ... 3 1 ⇒ 4, iPrompt yields the natural language explanation *Add the inputs*. By changing the input form of the data, we can generate explanations that accomplish different tasks from the example, such as: i) recovering a dataset explanation, ii) generating a prompt transferable between LLMs, and iii) proposing novel descriptions. iPrompt works by using a pre-trained

LLM to iteratively propose and evaluate different candidate explanations.

For evaluation, we curate a diverse collection of datasets written in natural language (Table 1) and measure iPrompt's ability to accurately explain a ground-truth pattern. We find that iPrompt outperforms baseline methods in accurately finding a correct description; moreover, the generated descriptions are interpretable, allowing human auditing and enabling strong generalization when used as a prompt in a new setting (i.e. when used for a different LLM). On real-world sentiment classification datasets, iPrompt even produces prompts that match or improve upon human-written prompts for GPT-3, while only using smaller, locally-run language models. Finally, we find that iPrompt is able to extract information from real-world scientific datasets.

2. Related work

Prompting and autoprompting. With the advent of large-scale models, prompting (i.e. finding the right prompt to use to query an LLM for a given task) has exploded as an area of inquiry, often yielding impressive improvements in performance (Brown et al., 2020; Petroni et al., 2019; Liu et al., 2021a) and spurring a line of work aiming to make prompting easier (Strobelt et al., 2022; Lu et al., 2022; Bach et al., 2022; Logan IV et al., 2022). Recently, autoprompting (i.e. automatically searching for a prompt or prompt-embedding via optimization) has emerged, with methods such as prefix-tuning (Li & Liang, 2021), P-tuning (Liu et al., 2021b), prompt-tuning with rules (Han et al., 2021), knowledgeable prompt tuning (Hu et al., 2021) and many more (Liu et al., 2021a). These strategies use gradient descent to find a set of "adapter" parameters that maximize model performance, but do not require that the new parameters map back to tokens in discrete space, rendering them uninterpretable.

A few methods tackle the more difficult problem of searching for prompts that can be expressed in natural language tokens. RLPrompt (Deng et al., 2022) searches for such a prompt using reinforcement learning and one recent work (Honovich et al., 2022) queries an LLM to produce a prompt. AutoPrompt (Shin et al., 2020) performs autoprompting via input gradients (see Sec. 3). Similarly, adversarial triggers (Wallace et al., 2019) use autoprompting to identify adversarial inputs which can be used to change a model's prediction. These methods effectively alter a model's predictions, but do not constrain the discovered prompts to be semantically meaningful, resulting in prompts that are difficult to interpret (Webson & Pavlick, 2021). Another related work directly finetunes an LLM to describe the difference between two datasets (Zhong et al., 2022). Concurrent work proposes a method for natural language prompting similar to the one here, with a focus on improv-

ing prediction performance rather than on explaining data patterns (Zhou et al., 2022).

Problems related to dataset explanation The problem statement presented in this work closely resembles the widely studied problems of symbolic regression (Augusto & Barbosa, 2000; Schmidt & Lipson, 2009), program synthesis (Gulwani et al., 2017; Manna & Waldinger, 1980), text/table summarization (Kryściński et al., 2019; Liu et al., 2018), and pattern discovery in data-mining (Hand, 2007). iPrompt can be viewed as an algorithm for symbolic regression, in which the set of allowable symbols consists of semantically meaningful natural language strings. One recent work proposes the task of inferring prompts that improve supervised prediction (Honovich et al., 2022), which we generalize here to diverse use cases for dataset explanation.

Alternative methods for neural-network interpretation A popular method for interpreting neural networks is to inspect an LLM's individual predictions via feature importances (Lundberg et al., 2019; Ribeiro et al., 2016), feature-interaction importances (Singh et al., 2019; Tsang et al., 2017), extractive rationales (Zaidan & Eisner, 2008; Sha et al., 2021), or natural language explanations for individual predictions (Hendricks et al., 2016; Camburu et al., 2018). These works can provide meaningful insights for individual predictions, but it is difficult to parse them into an understanding of an entire dataset. Alternatively, one can investigate whether an LLM's learned representations via probing (Conneau et al., 2018; Liu & Avci, 2019) or by directly analyzing a model's internal weights and activations (Wang et al., 2021; Olah et al., 2018; Meng et al., 2022). However, these approaches are limited in their ability to generate previously unknown descriptions of data. A different approach involves distilling information into a transparent model (Tan et al., 2018; Ha et al., 2021; Singh & Gao, 2022) or simply using a transparent model in the first place (Breiman et al., 1984; Tan et al., 2022; Singh et al., 2021; Agarwal et al., 2022).

3. Methods: Defining the task and approach

3.1. Task: Dataset Explanation

Given a dataset comprised of input-output string pairs $\{(x^1, y^1), \ldots, (x^N, y^N)\}$, the goal is to produce a "semantically meaningful" natural language string that explains the relationship between x and y. We require that a string consists of human-understandable text rather than a sequence of incongruous tokens. For example, in the dataset shown in Fig. 1, given samples of data performing addition, our task is to recover text synonymous to *Add the inputs*. This dataset explanation can then be used for various downstream tasks, such as prompting a different LLM.

Table 1. Dataset Explanation Tasks. Each collections contains # different task. Roman numerals correspond to the use cases in Fig. 1. For full details on each dataset, see Appendix A.2.

Collection	#	Description
1) Synthetic math	10	Mathematical functions (i), (ii)
2) Allen NLI	10	Language tasks (i), (ii)
3) Instr. induction	20	Language tasks (i), (ii)
4) Sentiment	4	Sentiment classification (i), (ii)
5) Proteins/chemicals	3	Protein/chemical properties (iii)
6) Language fMRI	20	Excitation of fMRI voxel (iii),(iii)

Datasets Table 1 shows the collections of datasets we study: (1) *Synthetic math* – datasets that require inferring an underlying mathematical function based on numeric input and outputs; (2) *Allen NLI* (ANLI) and (3) *Instruction induction* (Honovich et al., 2022) – diverse language tasks (Wang et al., 2022) with easily verifiable descriptions (e.g. *Find a country's capital*). (4) *Sentiment* – a collection of sentiment classification datasets in different domains. For collections (1-3), there is a ground-truth prompt available for evaluation. For example, when adding two numbers (Fig. 1), the rule checks whether a description contains any of the keywords *add*, *sum*, or +. We also study scientific datasets on (5) *proteins/chemicals*, and (6) *fMRI* with full details given in Sec. 6.

3.2. Approach: iPrompt

We now detail approaches for the general problem of autoprompting before introducing iPrompt, our method for interpretable autoprompting. We specify autoprompting as a discrete search problem. Given a dataset of n input-output pairs $\{(x^1, y^1), ..., (x^n, y^n)\}$ and a pre-trained LLM f that returns the log-probability of a given string, autoprompting finds a natural language explanation $\hat{s}$ maximizing:

$$\hat{s} = \underset{s \in \mathcal{S}}{\mathrm{argmax}} \sum_{i=1}^{n} f\left(\mathrm{render}(s, x^i, y^i)\right) \qquad (1)$$

The render function is a problem-specific function that renders a natural language string from the prompt s and each example in the dataset (x^i, y^i). We use $\mathcal{S}$ to indicate the set of fluent strings, under some notion of syntactic fluency. This constraint is used to ensure prompts are readable, and potentially generalize to downstream LLMs. Solving this search problem exactly is intractable.

A core assumption of this objective is that semantically accurate prompts lead a model to assign higher probability to the correct output. To check this assumption, we analyze four datasets from the inverse synthetic math collection that share common structure for the inputs and prompts. Each dataset admits a prompt of the form *Return the ___ of the inputs.*, then is given two input numbers and queried for the
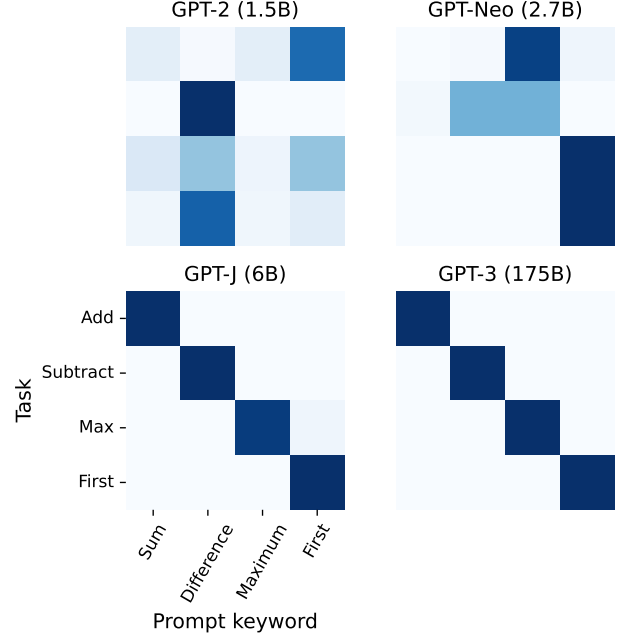

Figure 2. Prompt-based reranking depends on model size. Large models (GPT-J 6B and GPT-3) align prompts correctly to tasks. The model is given the prompt *Return the ___ of the inputs.*, where ___ is filled in with the shown prompt keyword before querying the output given two inputs numbers in a string. Darker indicates a higher accuracy, and high accuracy along the diagonal indicates that the correct prompt induces the highest accuracy.

output.

Fig. 2 shows the accuracy of different models at performing these tasks across different input prompts.[2] For small models, the prompts are unsuccessful, but for large models (GPT-J 6B and GPT-3), the model is accurate if and only if given the correct prompt.[3] This result suggests that, at least for large models, the search for a prompt that maximizes performance correlates well with the underlying task. We will see in Fig. 4 that dataset explanation depends on this ability.

Baseline: AutoPrompt AutoPrompt (Shin et al., 2020) targets the objective posed in Eq. (1) using a gradient-based local search. AutoPrompt searches for $\hat{s}$ following the gradients of the objective Eq. (1) with respect to individual tokens in $\hat{s}$. It discretely changes individual words in $\hat{s}$ and then checks whether or not the newly updated $\hat{s}$ improves the objective score. The use of gradients allows AutoPrompt to find an effective prompt $\hat{s}$, but makes it difficult to find answers that satisfy the fluency constraint $\mathcal{S}$.

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[2]The accuracy is normalized for each task using softmax in order to visualize the effect of differing prompts.

[3]For details on each model, see Table A3.

(i) Proposal

In: 3 1 Out: 4	Combine the numbers
In: 4 7 Out: 11	Return the output
In: 5 9 Out: 14	Sum in order
Prompt:	Compute the output

(ii) Reranking

Combine the numbers

Sum in order

Compute the output

Combine the numbers

(iii) Iterate with exploration

In: 5 5 Out: 10	Combine the **numbers**
In: 9 3 Out: 12	Combine the **arguments**
In: 1 8 Out: 9	Sum **the numbers**
Prompt:	Sum **all inputs**

Sum the numbers ✔

Sum all inputs
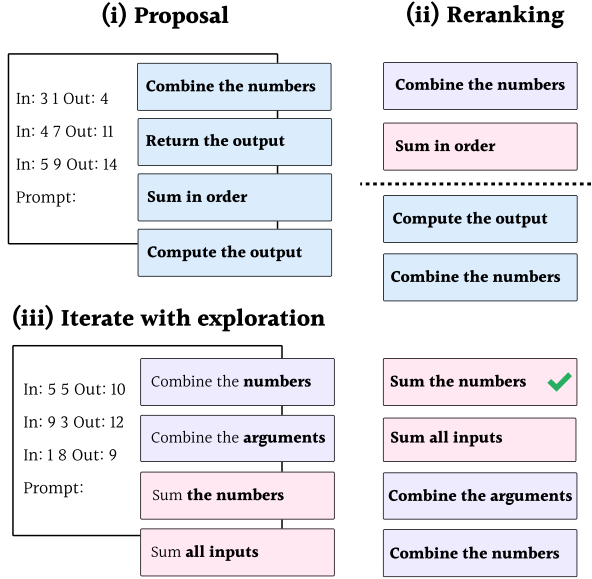
Combine the arguments

Combine the numbers

Figure 3. Overview of iPrompt. iPrompt first proposes candidate prompts, then ranks them based on their performance as a prompt, then truncates and regenerates them. This entire process is repeated until performance stops improving.

Baseline: Zero-shot suffix decoding LLMs themselves can be directly used to predict prompt strings. Following Honovich et al., we give the model a prompt string which contains data examples (e.g. *In: 2 5* x^i *Out: 7.* y^i *To compute the output from the input, ___,*) *template* and sample the output to recover a prompt $\hat{s}$ using nucleus sampling.[4]

Proposed method: iPrompt iPrompt (Fig. 3) is an iterative local search algorithm that alternates between three steps: (i) proposing candidate prompts, (ii) reranking candidate prompts, (iii) exploration.

(i) Proposal: Candidate prompts are generated by extending the zero-shot LLM generation. Given a data instance as a prefix, we sample a number of candidate prompts. The maximum length of each candidate is pre-specified and fixed. For example, in the add-two-numbers task (Fig. 3), we may generate four candidates: {*Combine the numbers, Return the output, Sum in order, Compute the output*}.

(ii) Reranking: Given candidates, the objective Eq. (1) is evaluated for each candidate prompt s. The top few candidates which maximize the objective are kept, e.g. narrowing down the candidates to {*Combine the numbers, Sum in or-*

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[4]We also consider averaging the model's output logits across all examples in the dataset before decoding the output, but find that it does not improve performance (see Appendix A.4).

der}.

(iii) Iterate with exploration: Each of the top candidates from reranking is truncated at a random position. These truncated candidates are used as a prefix when generating new candidate prompts via suffix decoding. For example, we may randomly select the start of the previous candidates and fill in the endings: {*Combine the ___, Sum ___*} → {*Combine the numbers, Combine both arguments, Sum the numbers, Sum all inputs*}.

The algorithm is repeated until identifying a suitably strong $\hat{s}$, e.g. *Sum the numbers*. Steps (i) and (iii) ensure that prompts remain fluent, while step (ii) improves the score of the prompts on the objective. Computationally, iPrompt only requires running inference on the pre-trained LLM, yielding a significantly lower memory requirement than methods such as AutoPrompt which require access to the LLM's gradients.

4. Experimental Setup

We consider two sets of experiments. First in Sec. 5, we explore iPrompt's ability to rediscover a correct and fluent prompt on the variety of simple instruction datasets (Table 1, top) with known answers. Experiments test the ability of the model to recover a known prompt while also remaining fluent in a way that generalize to human readers and to other language models. In Sec. 6 we apply iPrompt to scientific datasets (Table 1, bottom).

Language Models For the main set of experiments, we always generate prompts using GPT-J, a 6 billion parameter model (Wang & Komatsuzaki, 2021). We restrict prompts to {6,12} tokens for sentiment classification and 6 tokens for the remaining data collections in Table 1. For generalization experiments, alternative models are tested with the generated prompts including OPT and GPT-3 (Zhang et al., 2022; Brown et al., 2020). See Appendix A.4 for a full discussion of experimental details and Appendix A.3 for experiments on more models (e.g. Galactica (Taylor et al., 2022)) and more datasets.

Evaluation metrics We consider two types of evaluation: closeness to ground-truth and accuracy as a prompt. To measure closeness we use three metrics: (1) Correct – whether the generated explanation contains one of a set of problem-specific keywords. (2) MRR – Mean reciprocal rank measuring the rank of the first task-correct prompt. Given a set of datasets $\mathcal{D} = \{\mathcal{D}_1, ..., \mathcal{D}_N\}$, we compute: MRR $= \frac{1}{|\mathcal{D}|} \sum_{i=1}^{|\mathcal{D}|} \frac{1}{\text{rank}_i}$, where rank_i is the one-indexed rank of the first correct explanation. (3) Human – The human evaluation scores between the top-generated explanation and a pre-specified groundtruth explanation, when instructed "You are given a groundtruth description along

Table 2. Performance for dataset explanation. Dataset from Table 1 (1-3). Accuracy measured via (1) Human-evaluation (H, normalized %), (2) Mean Reciprocal Rank across the collection (M) and (3) 1-best correctness (C, %). For all metrics, higher is better.

	iPrompt H / M / C	AutoPrompt H / M / C	Suffix H / M / C
Math	**60 / 0.69 / 60**	25 / 0.14 / 13	20 / 0.08 / 03
ANLI	**56 / 0.41 / 37**	21 / 0.07 / 07	25 / 0.06 / 01
Induction	**42 / 0.35 / 28**	21 / 0.09 / 08	23 / 0.04 / 01

with a generated one. On a scale of 1 (worst) to 5 (best), how interpretable and accurate is the generated description?"[5]. The mean human evaluation score (ranging from 1 to 5) is normalized.

To measure generalization ability, we evaluate explanations based on accuracy as a prompt for other models. Accuracy is computed following (Brown et al., 2020; Raffel et al., 2020): using exact matching with beam search, a beam width of 4, and a length penalty of $\alpha = 0.6$.

For sentiment evaluation, we learn a prompt within the template *Input: "${input}"{prompt}*.[6] We use *positive* and *negative* as positive and negative labels and require the LLM to rank the two options. Human-written prompts are adapted to this template from open-source prompts available through PromptSource (Bach et al., 2022).

5. Results and Analysis

5.1. Dataset explanation recovery

Table 2 compares prompting methods across three diverse data collections. The *Human* evaluation scores are much higher for iPrompt than the baselines, suggesting that it finds prompts which are both accurate and human-interpretable. Similarly, the *MRR* and *Correct* scores show that iPrompt considerably improves in finding accurate explanations. See all generated explanations in Appendix A.3.

To assess the best-case absolute accuracy of the approach, we note it is impossible for the approach to recover the prompt if the underlying LLM cannot solve the task. Fig. 4 plots the prompt recovery performance (MRR) against the underlying LLM's accuracy (when using the groundtruth prompt) for each dataset. When the model can solve the task, iPrompt does well on recovery. However for many tasks the model has low accuracy even with the correct prompt, putting a ceiling on the performance of iPrompt.

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[5]Human evaluation scores are averaged over 4 PhD students in machine learning not affiliated with the study.

[6]In initial experiments, we find that performance drops significantly when learning a prompt that comes *before* the input.
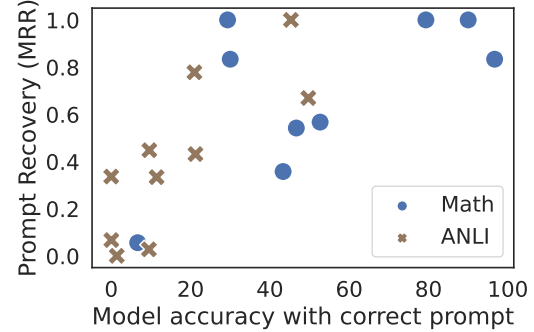

Figure 4. Comparison of model accuracy with correct prompt and iPrompt ability to find the correct prompt across each individual task (single-task MRR). Prompt recovery ability is dependent on the model's ability to perform the task.

Table 3. Generalization accuracy (zero-shot) with the prompts generated with GPT-J as the LLM across different models.

		Correct Prompt	iPrompt	AutoPrompt	No prompt
Math	GPT-J 6.7B*	54.0	**51.5**	41.6	16.3
	OPT 6.7B	12.7	**19.3**	**18.9**	8.4
	GPT 20B	76.1	**54.4**	23.2	8.5
	GPT-3 175B	76.0	**62.1**	40.8	28.4
ANLI	GPT-J 6.7B*	9.0	**4.7**	1.9	2.0
	OPT 6.7B	10.7	**6.7**	4.7	**7.9**
	GPT 20B	31.0	**14.2**	5.6	4.0
	GPT-3 175B	37.6	**11.7**	2.7	7.7

5.2. Generalization accuracy of prompts

Do prompts generated for a specific LLM still work when applied to a different model? Table 3 shows the generalization accuracy when testing the prompts generated using GPT-J (Table 5) on different LLMs. The prompts maintain effectiveness across most models. For the Math datasets, the iPrompt prompts elicit improvement over the baselines and approach the accuracy of the correct prompt. For the ANLI datasets, all prompts induce poor performance. Notably, the gap between iPrompt and AutoPrompt is larger for larger models (i.e. GPT 20B and GPT-3); this suggests that, by generating fluent prompts, iPrompt generates more generalizable descriptions.

Table 4 shows results on the sentiment analysis datasets. As prompts for GPT-J, iPrompt outperforms not only AutoPrompt, but also the manually-written prompt on all four datasets. Interestingly, the average performance of human-written prompts on GPT-J is very low, unlike the prompts generated by iPrompt. This indicates that models at 6B parameter scale may be brittle to the choice of prompt, even among a set of reasonable options, and iPrompt (and to an extent, AutoPrompt) is able to discover how to phrase prompts so that models of this scale can complete the task.

Table 4. Zero-shot accuracy on sentiment classification datasets: SST-2, Rotten Tomatoes, IMDB, and the Financial Phrasebank (Socher et al., 2013; Malo et al., 2014; Pang & Lee, 2005). Generation with GPT-J 6B and evaluation on both on the original GPT-J model and GPT-3 (`text-davinci-002`). Errors are standard errors of the mean.

		Human-written	**iPrompt**	AutoPrompt	No prompt
GPT-J	FFB	27.0 ± 1.9	$\mathbf{79.3 \pm 2.1}$	74.0 ± 9.1	47.5
	RT	58.9 ± 3.1	$\mathbf{84.8 \pm 0.9}$	73.0 ± 4.8	59.2
	SST-2	58.4 ± 2.8	$\mathbf{86.7 \pm 1.0}$	76.7 ± 3.9	60.9
	IMDB	66.0 ± 3.2	$\mathbf{87.9 \pm 1.4}$	86.7 ± 1.2	58.6
GPT-3	FFB	39.6 ± 1.6	$\mathbf{57.2 \pm 6.9}$	28.2 ± 3.1	39.1
	RT	$\mathbf{82.7 \pm 3.3}$	77.4 ± 2.8	57.8 ± 3.5	54.8
	SST-2	$\mathbf{90.5 \pm 3.9}$	82.4 ± 2.3	61.8 ± 7.0	58.4
	IMDB	75.6 ± 3.3	$\mathbf{86.6 \pm 1.1}$	70.0 ± 6.5	66.2

When sentiment prompt generalization is tested on GPT-3, we find that iPrompt prompts outperform human-written prompts on two of the four datasets. When tested on GPT-3, iPrompt prompt *To summarize this review! :* outperforms all PromptSource IMDB prompts that use the same verbalizer (*positive/negative*). When its prompts are tested on GPT-3, baseline AutoPrompt only slightly outperforms testing with no prompt at all.

Table 5 shows the top-ranked explanation generated by each method for selected datasets. iPrompt often finds an explanation that is indicative of the underlying relationship, even if the phrasing is not perfect. For example, for the *add two numbers* dataset, it finds *Create a function named 'sum.* The prompts found by iPrompt also read as fairly fluent strings compared to AutoPrompt, which produces an incoherent set of tokens.

5.3. Model ablations

We run ablation experiments to analyze the three steps of iPrompt: (1) Proposal, (2) Reranking, and (3) Iteration. we use the Math and ANLI datasets and run on a maximum of 5000 data points using 5 shots in context for prompt generation.

(1) *Proposals* are partially guided by examples. During the proposal stage, iPrompt prefixes potential prompts with dataset examples. Table 6 considers variants of this stage that remove input and output examples during the proposal stage. Note the system still has access to the full examples during the reranking stage. We find the system can achieve decent performance on Math simply by iterating. However for ANLI, the model needs to at least see the inputs/outputs during the proposal in order to find accurate prompts.

(2) *Reranking* zero-shot recovers better prompts. iPrompt uses zero-shot accuracy to rank prompts. As we

have examples of the task, we could instead use in-context few-shot prompting for ranking. Prior work suggests that prompt wording is less influential as the number of in-context examples increases (Webson & Pavlick, 2021). Table 6 shows that using these examples in-context for reranking does, in fact, considerably hamper prompt recovery. We further find that the LLM used for reranking is more important than the LLM used for proposals (see Appendix Fig. A3).

(3) *Iteration* improves performance Finally, Table 6 shows that without multiple iterations, performance drops nearly to zero (Fig. A2 shows more details on loss as a function of iterations).

6. Scientific investigations with iPrompt

We now investigate whether iPrompt can explain patterns in scientific datasets. Specifically, we analyze the Galactica model (Taylor et al., 2022) with 6.7 billion parameters. We query whether it can describe differences in datasets of chemical compounds and protein sequences before investigating a neuroscience problem.

Toxic chemical compounds We first ask whether iPrompt can explain the difference between two groups of chemical compounds with a known difference. We use the Tox21 dataset (Richard et al., 2020) which contains toxicity measurements on 12 biological targets. For each of the 12 biological targets, we search for a prompt that differentiates compounds that are toxic to the target (positive) from those which are not toxic to any of the targets (negative). We use 100 positive/negative examples for each biological target and format each input with the text *Here is a compound:\n [Compound Name]\n Answer:* followed by *Yes* for a positive compound and *No* for a negative one. iPrompt is run for a single epoch with 5 shots in each example.

Ideally, the elicited prompt would mention toxicity. Table 7 shows results for whether the elicited prompts contain the substring *tox*, both in terms of MRR and top-prompt correctness. iPrompt often finds an accurate prompt: one representative example is: *Answer yes if the compound is toxic, and Otherwise answer NO.* To ensure that this substring is not simply a popular completion for the language model, we compare against a baseline which runs iPrompt using Galactica proposals from empty inputs/outputs and reranking with Galactica; over 36 random seeds, *tox* appears in any generated prompt.

Differentiating protein sequences We turn to whether iPrompt can explain the differences between two groups of proteins. We use protein sequences and keywords from Swiss-Prot (Bairoch & Boeckmann, 1991) (a high-quality subset of Uniprot (Consortium, 2015)) to construct two

Table 5. Examples of generated explanations by iPrompt and AutoPrompt. See all prompts in Appendix A.3.

	Human-written prompt	**iPrompt**	AutoPrompt
Math	Return the sum of the inputs	Create a function named 'sum	¿:Returns Adding togetherFont accomplish
	Return the square of the input	Input number and return its square	Cal impl qApplySquare fiat
	Differentiate between prime/non-prime integers	Are these pairs of integers prime	ropheospels&& Norestricted
ANLI	Differentiate vegetarian/non-vegetarian foods	Are you a vegetarian?	compliedthe whether methamphetamine provided comp
	Differentiate the subject in a sentence based on gender	Predict the gender (F =	¡ endoftext ¿ -¿ M Fundamental FG Fav
	Return a synonym	what is a synonym for	Word termOn English meanings
	Translate english to spanish	please write English meaning in Spanish	the ththebb volunt
	Return a country's capital city	Which city is the capital and	Ang Suppose AUTHthe beh Assassins
Sentiment	What is the sentiment expressed by the reviewer for the movie?	Describe what it is about this film has caused it	Pap Azerb Saiyan Forean Talatar Yemeni IndBloomberg receiveda
	How does the author of the news headline feel?	<input> neutral> The result was due to: "	Fur resultolandgroundur augmented=

Table 6. Algorithmic ablations for each stage of iPrompt. Gives prompt recovery (MRR) achieved by ablating each stage. Averaged over 3 random seeds.

		MRR Math	ANLI
	iPrompt	**0.557**	**0.278**
(1) Proposal	w/o inputs+outputs	0.400	0.015
	w/o inputs	0.463	0.244
	w/o outputs	0.539	0.255
(2) Reranking	w/ in-context examples	0.071	0.152
(3) Iteration	No iteration	0.075	0.050

Table 7. iPrompt performance at recovering prompts for toxic chemical compounds. Tox21 results are averaged over 12 datasets with 3 random seeds each. Null data is averaged over 36 random seeds. Error bars are standard error of the mean.

	iPrompt	Baseline
MRR	0.83 ± 0.04	0.0
Top-prompt correctness	0.67 ± 0.08	0.0

Table 8. iPrompt performance at differentiating protein sequences. For both the *Cyto* and *Binding* datasets, the correct keywords are succesfully identified better than for the Baseline. Results are averaged over 12 random seeds; error bars are standard error of the mean.

	iPrompt (Cyto)	iPrompt (Binding)	Baseline
MRR	0.2 ± 0.08	0.08 ± 0.04	0.03 ± 0.01
Recall @ 5	0.25 ± 0.13	0.17 ± 0.11	0.05 ± 0.05
Recall @ 20	0.83 ± 0.11	0.33 ± 0.14	0.23 ± 0.09

shows results for identifying whether the elicited prompt contains one of the relevant keywords for each dataset (e.g. *Cytoplasm*). Despite the difficult input format, the correct keywords are successfully identified for both the *Cyto* and *Binding* datasets better than for the *Baseline* (which again contains empty inputs).

Scientific investigation into an fMRI natural language dataset We now explore using iPrompt in a simple neuroscience experiment. A central challenge in neuroscience is understanding how and where semantic concepts are represented in the brain. A recent seminal study (Huth et al., 2016) explores this question by investigating where different natural language categories are represented in the human neocortex. Specifically, the authors collect functional MRI (fMRI) responses as human subjects listen to hours of narrative stories. They then build a predictive model of these responses for each voxel (i.e. a small region in space) in the brain, which takes as input the words contained in the stories (and other features). To interpret these individual voxel models, they cluster the words in the narrative stories into 12 groups and manually annotate them, resulting in 12 categories, such as *tactile*, *visual*, and *professional*. Finally, they view the spatial mapping of these 12 concepts (projected onto low dimensions) across the brain using their individual voxel models.

We revisit a small piece of this study's analysis through

datasets: each dataset contains two groups of proteins, which are differentiated based on their keywords.[7] The first dataset, which we call *Cyto*, has proteins with either the keyword *Cytoplasm* or *Membrane*. The second dataset, which we call *Binding*, has proteins with either the keyword *RNA-binding* or *ATP-binding*. Each group is randomly downsampled to 100 proteins and iPrompt is run with the same hyperparameters as when finding chemical compounds.

We make this problem more challenging by feeding the model the raw protein sequence (not the protein name) which ranges from hundreds to thousands of amino acids. Each input is presented with the following text: *Here is a protein sequence:\n [Protein Sequence]\n Answer:* followed by *Yes* for a one group and *No* for the other. Table 8

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[7]We search for reasonably popular but non-cooccuring keywords in the proteins; see details in Fig. A5

the lens of iPrompt. Specifically, we ask whether iPrompt could generate plausible categories that are well-represented across the brain but differ from the manually identified 12. We fit a predictive model for each voxel, following the pipeline of the original study (details in Appendix A.6). We then use the resulting models to identify a list of the top-15 words which most excite each voxel. For example, the top-15 words that excite the best-predicted voxel are: *sheet, edges, diameter, strips, cardboard, copper, steel, colored, coloured, leaf, wire, cap, paper, shaped, tin*. To identify a plausible semantic category, we construct a template string as follows: *The following list of words all belong to the same semantic category: ___\n\n sheet, edges, ..., shaped, tin*. We then use iPrompt (again with a GPT-6B parameter model) to generate a category by filling in the blank (restricted to a single token). To make iPrompt more effective, for each voxel we use iPrompt on a set of examples consisting of 15 permutations of the top-15 words, allowing finding patterns that are not overly sensitive to the word-ordering.

Given the top categories for each voxel, we analyze the mapping of recurring categories across the neocortex. We aggregate the top-15 inferred categories[8] over the top-15 best-predicted voxels and find that the most frequently inferred categories are: `material, color, surface, text, & fabric`. Interestingly, these are sensible quantities that different voxels could reasonably be selective for. We spatially map each of these identified categories (e.g. *material*) across the 10,000 best-predicted voxels by using the LLM in a second way. For each voxel, we condition the LLM (again GPT-6B) on the top-15 words list, and evaluate the predicted probability for each category, i.e *The following list of words all belong to the same semantic category: sheet, edges, ..., shaped, tin The semantic category they all belong to, in one word, is ___*. The higher this predicted probability, the more selective we infer that a voxel is for the category. Fig. 5 shows these predicted probabilities for the top-two inferred categories (*material* and *color*) across the cortex of a human subject.

While there is no groundtruth for this semantic map, one noteworthy feature of the resulting map is that it is spatially smooth (quantitatively, Fig. A8 shows that the variance of the map among neighboring pixels is significantly lower than we would expect by shuffling the map's values). This is non-trivial, as nowhere in the modeling process was spatial information incorporated: each voxel was modeled independently and the displayed prediction was queried independently. We expect the underlying map to be smooth, both due to local connectivity in brain regions and also because the BOLD signal measured by fMRI does not have perfect spatial resolution. Thus, the fact that our inferred map is

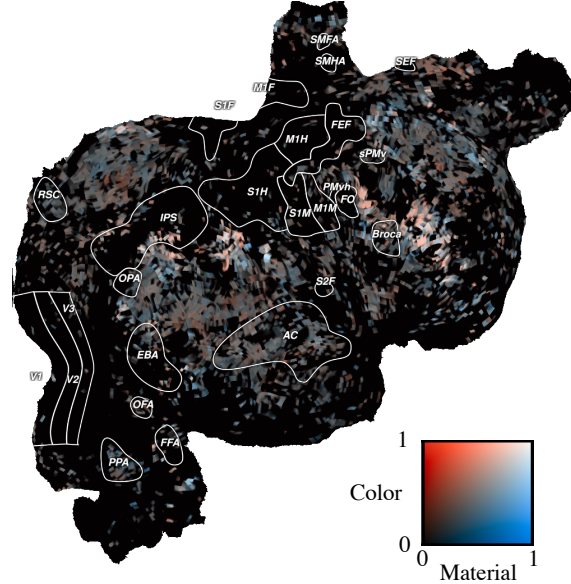[8]We apply stemming and remove stopwords before choosing the best categories.

Figure 5. Representations of the iPrompt-elicited concepts *material* (blue) and *color* (red) across the surface of the neocortex are spatially clustered and smooth. Only the top 10,000 best-predicted voxels are shown, remaining voxels are shown in black. Only the right hemisphere is shown (see both hemispheres, which show consistent smoothness in Fig. A6).

smooth suggests that (i) something about these categories is genuinely captured by the representation in the human brain, and (ii) that the iPrompt approach was able to reflect at least some of it. Beyond the two categories shown, the five categories generated by iPrompt exhibit spatial smoothness across the neocortex (Fig. A8).

7. Conclusion and Discussion

iPrompt makes a meaningful step towards finding natural language prompts that are both accurate and human-interpretable. We show this method can be used to recover dataset descriptions, produce transferable prompts, and provide explanations for experimental data. One future direction could elicit *targeted* information from data via the use of a *template*. For example, one may use iPrompt to extract feature importance by prepending the learned prompt with the string "To get the answer from the inputs, the most important inputs are ___". As another example, in a scientific study such as the fMRI study in Sec. 6, a scientist interested in a particular topic (e.g. *fear*) may investigate that particular topic by making a more specific template (e.g. *How are these words related to the concept of "fear"?*).

While we focus on text, iPrompt could be applied generally settings where an LLM performs well. For example, in computer vision, an interpretable autoprompt may look like a mask of an image, and in vision-language models, an interpretable prompt may be a description of a vision task,

e.g. *find the largest shape in this image.*

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A. Appendix

A.1. Sentiment classification results

Table A1 shows the best prompt produced by each method for each sentiment dataset. iPrompt often learns to recreate significant examples from the dataset, as a prompt. Figure A1 shows loss across training step for each method and dataset, across three random seeds. We see that AutoPrompt often finds a prompt with slightly lower loss on the training data, although its prompts lead to worse generalization, as reported in Table 4. Each training step represents a single word swap (in the case of AutoPrompt) or the truncation and generation of a new prefix (in the case of iPrompt).

Different from the other experiments in this paper, for sentiment classification, we initialize AutoPrompt with random tokens instead of all *the*, as we find AutoPrompt fails to find an effective solution for longer prefix lengths when all tokens are initialized to *the*. To accommodate for a complex input-output relationship, we test prompts of length 12 as well as length 6.

Accuracy is measured on the test set when available; otherwise, it is measured on a held-out 25% of the train set.

Table A1. Best-of-three prompts generated by each method on sentiment classification datasets. (Human-written prompts are best-of-eight and take from PromptSource (Bach et al., 2022)).

| Task	Method	Prompt
Financial phrasebank	AutoPrompt Human-written prompt iPrompt	Fur resultolandgroundur augmented How does the author of the news headline feel? <input> neutral> The result was due to: "
IMDB	AutoPrompt Human-written prompt iPrompt	uclear cend Koretravel NAACP curses SicAstings production received The movie review in negative/positive sentiment is: This movie needs to be put up on my profile as my
Rotten Tomatoes	AutoPrompt Human-written prompt iPrompt	Whether{{ anotherath¡—endoftext—¿ how What sentiment does the writer express for the movie? what words would you try to add to help you express that
SST-2	AutoPrompt Human-written prompt iPrompt	BryceSpecificallyWASHINGTONRatedam What is the sentiment expressed in this text? It is clear from the sentence that all three actors have something
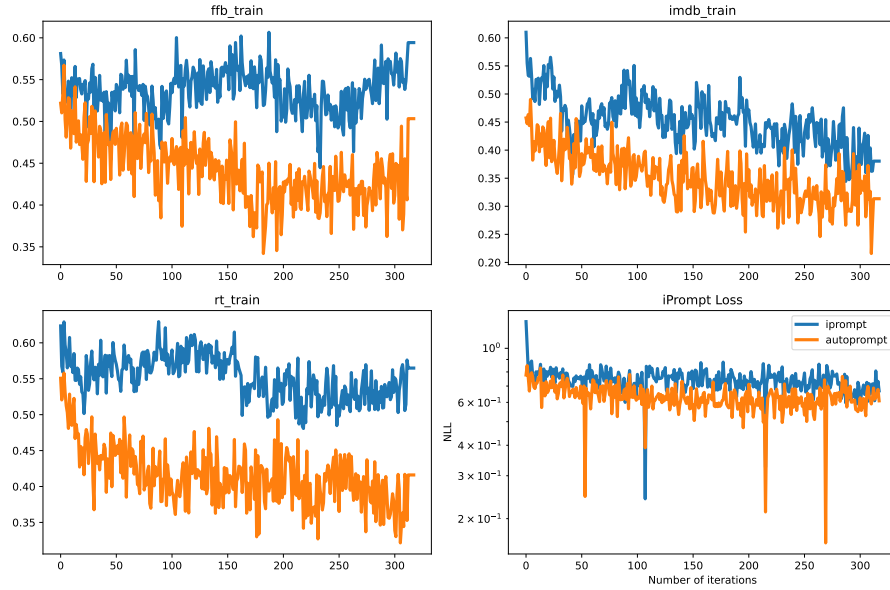
Figure A1. Loss plots for methods across sentiment analysis datasets, showing AutoPrompt and iPrompt across three random seeds.

A.2. Data/model details

Table A2. Details for each dataset. For details on *Instruction induction*, see (Honovich et al., 2022) and for details on *Distribution differences*, see (Zhong et al., 2021).

Task name	Samples	Description	Example
fibonacci_one	10	Given an input x, return the xth fibonacci number.	Given the input x is 8, the output f(x) is 21.\n\n
double_one	10	Given an input x, return 2*x.	Given the input x is 6, the output f(x) is 12.\n\n
exp_one	10	Exponentiate the input to get the output.	Given the input x is 8, the output f(x) is 2980.96.\n\n
square_one	10	Square the input to get the output.	Given the input x is 2, the output f(x) is 4.\n\n
first_two	100	Return the first of the inputs.	Given the input numbers 7 and 8, the answer is 7.\n\n
add_two	100	Return the sum of the inputs.	Given the input numbers 9 and 7, the answer is 16.\n\n
subtract_two	100	Return the difference of the inputs.	Given the input numbers 5 and 4, the answer is 1.\n\n
divide_two	100	Return the quotient of the inputs.	Given the input numbers 2 and 7, the answer is 2/7.\n\n
multiply_two	100	Return the product of the inputs.	Given the input numbers 3 and 3, the answer is 9.\n\n
max_two	100	Return the maximum of the inputs.	Given the input numbers 1 and 1, the answer is 1.\n\n
task1191_food_veg_nonveg	101	Return whether the input food dish is vegetarian (yes or no).	Input: Haq Maas Answer: no\n
task1149_item_check_edible	119	Return whether the input item is edible (yes or no).	Input: vase Answer: no\n
task1146_country_capital	231	In this task, you are given a country name and you need to return the capital city of the given country	Input: Saint Pierre and Miquelon Answer: Saint-Pierre\n
task1147_country_currency	232	You are given a country name and you need to return the currency of the given country.	Input: Senegal Answer: CFA Franc BCEAO\n
task1509_evalution_antonyms	551	In this task, you are given an adjective, and your job is to generate its antonym. An antonym of a word is a word opposite in meaning to it.	Input: paper Answer: scissor\n
task183_rhyme_generation	999	Given an input word generate a word that rhymes exactly with the input word. If not rhyme is found return "No"	Input: think Answer: sync\n
task107_splash_question_to_sql	2031	In this task you are expected to write an SQL query that will return the data asked for in the question. An SQL query works by selecting data from a table where certain conditions apply. A table contains columns where every row in that table must have a value for each column. Every table has a primary key that uniquely identifies each row, usually an id. To choose which columns are returned you specify that after the "SELECT" statement. Next, you use a "FROM" statement to specify what tables you want to select the data from. When you specify a table you can rename it with the "AS" statement. You can reference that table by whatever name follows the "AS" statement. If you want to select data from multiple tables you need to use the "JOIN" statement. This will join the tables together by pairing a row in one table with every row in the other table (Cartesian Product). To limit the number of rows returned you should use the "ON" statement. This will only return rows where the condition...	Input: What are the order ids and customer ids for orders that have been Cancelled, sorted by their order dates? Answer: SELECT order_id , customer_id FROM customer_orders WHERE order_status_code = "Cancelled" ORDER BY order_date\n
task088_identify_typo_verification	6499	The given sentence contains a typo which could be one of the following four types: (1) swapped letters of a word e.g. 'niec' is a typo of the word 'nice'. (2) missing letter in a word e.g. 'nic' is a typo of the word 'nice'. (3) extra letter in a word e.g. 'nicce' is a typo of the word 'nice'. (4) replaced letter in a word e.g 'nicr' is a typo of the word 'nice'. You need to identify the typo in the given sentence. To do this, answer with the word containing the typo.	Input: A laege display of apples, pears, and oranges Answer: laege\n
task1336_gender_classifier	6500	Return the gender of the person in the input sentence.	Input: Justin made me feel discouraged. Answer: M\n
task092_check_prime_classification	6500	In this task, you need to output 'Yes' if the given number is a prime number otherwise output 'No'. A 'prime number' is a a whole number above 1 that can not be made by multiplying other whole numbers.	Input: 9319 Answer: Yes\n

Table A3. Models analyzed here.

Model name	Huggingface identifier	Citation
GPT-2 (1.5B)	gpt2-xl	(Radford et al., 2019)
OPT (2.7B)	facebook/opt-2.7b	(Zhang et al., 2022)
GPT-Neo (2.7B)	EleutherAI/gpt-neo-2.7B	(Black et al., 2021)
Flan-T5 (3B)	google/flan-t5-xl	(Chung et al., 2022)
GPT-J (6B)	EleutherAI/gpt-j-6B	(Wang & Komatsuzaki, 2021)
OPT (6.7B)	facebook/opt-6.7b	(Zhang et al., 2022)
Galactica (6.7B)	facebook/galactica-6.7b	(Taylor et al., 2022)
GPT-Neo (20B)	EleutherAI/gpt-neox-20b	(Black et al., 2022)
GPT-3 (175B)	text-davinci-002 (OpenAI API)	(Radford et al., 2021)

A.3. iPrompt results extended

We consider discriminators of varying sizes, with GPT-J (6B) as a prompt generator. We also compare generators of varying sizes with GPT-J (6B) as a prompt discriminator. Models considered are of $\{125M, 1.3B, 2.7B, 6B\}$ parameters from the GPT-Neo/GPT-J language model family. Results are shown in Fig. A3. Performance varies smoothly across model sizes, with the highest performance when using the largest model for both reranking and generation. Reranking appears slightly more important than generation. When using a 1.3B parameter model for generation, MRR drops only slightly, from 0.418 to 0.399, while when using a 1.3B parameter model for reranking, MRR drops to 0.211. In general, prompt recovery performance improves smoothly with reranking model size.

Fig. A2 plots the progress of iPrompt across iterations, comparing runs on Math datasets (blue) to runs on ANLI datasets (gray). iPrompt appears to make most of its progress during the first 20% of training and then continue to slowly decrease the average loss. Running for more iterations on additional datapoints would likely increase performance.
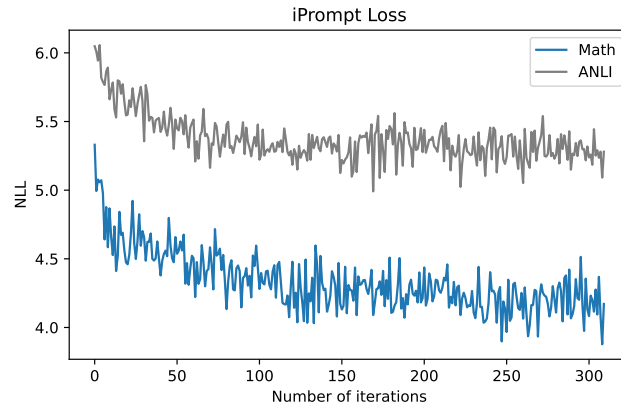
Figure A2. iPrompt performance across training, averaged across three random seeds and all tasks from Math datasets (Blue) and ANLI (Gray).
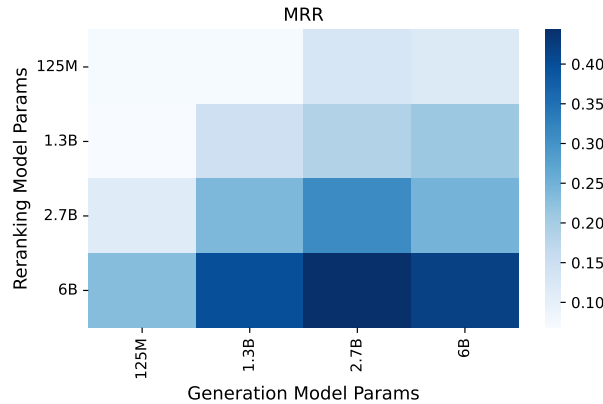
Figure A3. iPrompt performance across different size language models for the prompt proposal and reranking steps. Values are mean reciprocal rank of first accepted prompt averaged across 20 tasks and 3 random seeds.

Table A4. Performance of Galactica at prompt recovery, including DD datasets (Zhong et al., 2022; 2021).

		iPrompt	AutoPrompt	Suffix
MRR	Math	**0.2**	0.09	0.025
	ANLI	**0.39**	0.0025	0.085
	Induction	**0.14**	0.098	0.056
	DD	**0.064**	0.0082	0.066
Correct	Math	**0.12**	0.075	0
	ANLI	**0.34**	0	0.025
	Induction	**0.071**	0.087	0.02
	DD	**0.043**	0	0.052
BLEU-Top Prompt	Math	**0.0073**	0	0
	ANLI	**0.01**	0	0.00032
	Induction	**0.022**	0	0.0027
	DD	**0**	0	0.0015

Table A5. Examples of top-generated prompts for each method: GPT-J main datasets.

	autoprompt	iprompt	suff
active to passive	(= 18 the the subst	Choose a pronoun for each sentence	Create a sentence or group of
add two	>:Returns Adding togetherFont accomplish	Create a function named 'sum	n>2 m1
antonyms	the bectheBut But	The noun to its opposite (	The code to ascend. You
cause and effect	REG Kinect virginity developed mosquit The	What would each sentence be if	write programs that read through an
common concept	???????? parted configuredthe ????????	Find a noun that includes all	which is a common word used
diff	""Fair 62 disgust 92 81	Find the difference between largest	Write a program or function to
divide two	soughtWomen surgicalthe Percentage treated	"Divide each digit by	write a program or function who
double one	says transit Farethe doubles dollars	Write a function called double_	Given two function pointer A and
exp one	&&wl +# 123 270 Earthquake	Input this into your calculator (	Type in number between 15 &
fibonacci one	baptpi produce347).''	Implement a function to find Fib	Given an integer n (1
first two	Binding decode wr detect shortest numeric	Find first digit of given number	When was Python added to Ubuntu
first word letter	Exception Ps< endoftext >the the	Make a program that reads in	nimshul, a
informal to formal	CLASSIFIEDthe themselves strongly Plays Chamber	These are questions on simple sentences	Make the following sentences positive stateme
larger animal	????????thethethethethe	What is the most common animal	dogAnswer to "What's
letters list	fluidsthethethethethe	Given the following list of tokens	The computer will make this document
max two	spendingthethethethethe	Implement a version of max()	Write code to find out given
multiply two	ruits="# multipl integer multiplied False	'How do you multiply a	write a program or function who
negation	performs antiv Sizethe NULL NULL	I found these four mistakes below	Your friends think that you
num to verbal	irritatedthedd respectfully Protectivethe	Output each number below in the	The program outputs the first input
orthography starts with	nextbusiness wordevery morphpp	Name of two homophones	You will be given five words
rhymes	Steal batter dating: unfold testosterone	Find the missing word for all	Input [create] What
second word letter	i mascot okay kk	Who gave the answer "o	the United states government outlawed
sentence similarity	value %%%% Math	3 (5 marks). The	Read five sentences about your topic
sentiment	positively optimistic&&&& negative	I'm voting "negative"	Melvins at CBGB
singular to plural	Enhanced shorthand Lets pluralbetweenthe	Given a noun and its plural	1. It may be
square one	Cal impl qApplySquare fiat	Input number and return its square	Write a program or function to
subtract two	ignorethethethethethe	Write a function to find difference	Given a non-negative integer
sum	Photosthethethethethe	Add two numbers together and then	The program outputs, without any
synonyms	Word termOn English meanings	what is a synonym for	Is there a cure for an
task088 identify typo verification	thethethethethe	This word scramble is to test	You wake up in the morning
task092 check prime classification	ropheospels&& Norestricted	Are these pairs of integers prime	Print the input numbers in order
task107 splash question to sql		How Do You Connect SQL To	To get into MySQL you first
task1146 country capital	Ang Suppose AUTHthe beh Assassins	Which city is the capital and	France, England or the UK
task1147 country currency	aaaathecurrency Nib Sc	Ireland. Which currency is spoken	"I am working on a
task1149 item check edible	no the870830 yes	coffee and beans are fruits.	Which one of the following is
task1191 food veg nonveg	compliedthe whether methamphetamine provided comp	Are you a vegetarian?	It could be any food,
task1336 peixian equity evaluation corpus gender classifier	< endoftext > -> M Fundamental FG Fav	Predict the gender (F =	??????,???,
task1509 evalution antonyms	contrad orously inverted ironically trans	find words with the opposite meaning	Record your input and answer,
task183 rhyme generation	quarterdream dug}. Thro rhy	Mind vs Glee! There	what do you love to eat
taxonomy animal	programmingQ errorsBefore admitting mont	What are the most common animals	Each of these questions is a
translation en-de	H prob Hyper Forthe	You are a lawyer practicing in	This is an example of input
translation en-es	the ththebb volunt	please write English meaning in Spanish	Porque?
translation en-fr	IRthe< endoftext >thethe the	What is the French word for	Your code needs to deal with
word in context	("nSame distinguishedthethe	Same and Not-Same -	What you will do is have

Table A6. Examples of top-generated prompts for each method: GPT-J DD datasets (Zhong et al., 2022; 2021).

	autoprompt	iprompt	suff
d3 0		line contains this string? No	contains all 6 items, No
d3 1	Ghostbustersthe interrogation condition criminall	sentence contains "yes" or	string doesn't match any template
d3 10	preceded Roosevelt nonexistentuphem_-_ Tw	message contains "no". No	contains all of these words or
d3 11	caused senator prompt Recall interacted	string contains "No" or	was matched; output otherwise No
d3 12	begin:" r "},{" contradict	tweet mentions yes	is true or output false if
d3 13	},{" vote [*]=>	answer "no" (or	contains all correct answers, No
d3 14	nonexistent undead questions Enhance mandated no	string begins 'no' and	string contains any non blank white
d3 15	rarely ----Question not},{" geometric	string contains "no" or	includes exactly two English words with
d3 16	\n pearthemar Display RUN	text contains any "yes".	text is true, otherwise write
d3 17	EMP Similarly\t=== charsthe	is an answer ("no",	contains all correct answers for this
d3 18	\n\n Verb horm suffix Eucl	phrase starts with 'no',	contains all correct answers else No
d3 19	\n."," Emacs strips colors strips	word starts with 'yes',	text contains any of these strings
d3 2	indirectly [[pervasive?"Spoiler exhaustive	ends with "yes". If	sentence has an "O"
d3 20	\n\n dips Vote flower Ainthe	ted sentence contains both "yes	contains one of these words or
d3 21	\nthePubLeft Abstract	ends with 'no'. No	contains all correct answers, or
d3 22	Nov wholesno Eucl NO	can output no/yes,	data set contains results for output
d3 23	vantage immediately recogn example nails 309	no else output none? Input	contains data describing or referring to
d3 24	noBER nonosRew [	datum defines finite number fields	is in fact equal 2;
d3 25	withdrawalsnob inher nob Among	contains both gene list data file	has already started in state x
d3 26	Joined robberHigthe contradictionNarr	line ends with a space,	ted series matches any of these
d3 27	verseoleon:- inferred cannabinoids	was positive answer and "No	string of words, as shown
d3 28	\n repet999 REM=[nov	refers exclusively (only literally or	was a real question that could
d3 29	\n Pat uncertaintiesMerit oppos	line begins with yes	text meets any one or more
d3 3	\n\n887odynamHor mun\t	ends with "yes" and	statement reflects truth. Otherwise output
d3 30	detainees gap ${. hardness	statement is false? Otherwise	is an example from each category
d3 31	\n055 helium **** itching	phrase does not contain any words	given was false or not a
d3 32	Afghthethethe	matches either one of these strings	text is true, and write
d3 33	le \r 253	has a duplicate word. Correct	contains yes
d3 34	the Carnegie allerg Qu the	no,no for (1	was "The End" or
d3 35	Hatch Land pri poker[[Yah	would be a no (I	text can create a good argument
d3 36	], egregbyte?Sensor	matches exactly a "no".	string meets any, or exactly
d3 37	noun441...? word first neg	question has an answer "no	string meets any, and write
d3 38	wond <+ HELP"},{"InvalidOtherwise	says yes	"yes" has an
d3 39	notnobbutthe but	reads like no.	answers "yes" for all
d3 4	\n\n 760 consensualNarr Fog cabbage	sentence ends with "no".	string was a valid answer otherwise
d3 40	modeXP/, \n but	question contains an actual "no	given was wrong or not relevant
d3 41	opinions universitythe began followingawaru	sentence is grammatically correct,	equals to zero (i.
d3 42	disqualified hemor Ratings [contradiction Moham	phrase represents something that is actuallyhas 1 out of 2 responses
d3 43	\n\n saturated Phot misc	would be rightAnswer :no	was about a government regulation (
d3 44	\n <[npm spaces1	was "no": Input	was "yes" else false
d3 45	\n\n pit VerbFalse Tok	string contains one "no".	text starts with "OK",
d3 46	},{" Neil kingthe	no when a string containing one	contains this string! Yes,
d3 47	network intuitive 19 Lamp	sentence implies that no can mean	contains all digits, else No
d3 48	nond307 Literally negativeJun corpor	conforms with known facts no	ted number from user base 5
d3 49	Falsethe Rect 802	string contains "no" or	contains all of these words,
d3 5	contradicts absurdity Luffythe neg answ	string 'no' appears as	is correct ; No otherwise
d3 50	_____ WithNo","hedon	mentions "no" (or	contains all correct items, No
d3 51	\n\n 276WithNo noodles Cosponsors	reads "no" no else	given was no; not output
d3 52	\n\n 225Should laure	string was 'no' and	string contains just one space.
d3 53	never_{ Johns neo no	is all lower case answer 1	was what I described above!
d3 6	forbids Literally reminisNone negate	text contains any "no"	text contains Syrian
d3 7	},{"\r stringologically $\ git	contains 'no' or output	text contains yes
d3 8	unlikelyEitherselessletter Ches contradictory	sentence contains 'no' or	contains any newlines after matching
d3 9	reactive happensMiddle lot Inc	matches any word (no is	text meets any, or none

Table A7. Examples of top-generated prompts for each method: Galactica main datasets.

	autoprompt	iprompt	suff
active to passive	Transmission Electthe chromosome initialized empl	4-way Multiple Choice	Is the context a good response
add two	addthe Hyper addi	In order to add two or	Given three real-valued inputs
antonyms	meet equilibration stiptertead asymmetry	What is the opposite of each	[T1] Question
cause and effect	shaking Dthethethethe	Find clues as to why each	What do you think will happen
common concept	Bary techntbltbltbl Te	Where are all the animals?	What's the most common
diff	quartic digits shorter recreational genomics	Given two positive integers a and	What's the most efficient
divide two	manipulations comput iterationects quotients	The ratio of two real or	Given two different positive integers what
double one	roll Add Pingthe brakingthe	Determine how much money did Al	What's it like to
exp one	visc poplLSPLC Viscositythe	Given a number y and an	Find a formula for this linear
fibonacci one	start Attstrass Prim Polynomial emotions	\bigcirc m o	Write a function that gives an
first two	AICthethethe Adethe	Solve using negative exponents? Explain	We have found it helpful to
first word letter	d rthe l c syllable	What is the last word?	the program {x.
informal to formal	Why unpredictable comprobablyould Detecting	Yes! However, since we	Text-to-Text Data
larger animal	sharkoganopeanionaller descri	A question is given about three	Is the pair of animals on
letters list	microm phon te photothermal te te	How many 8 letter words	Given the following paragraph, indicate
max two	$$amater Penet credible b	How large was each of your	Is that as simple or complex
multiply two	aris visualthe Gibson multiplicative lexical	When we multiply two even or	What number divided by what other
negation	brood he Apparent denselythe FIG	What did these people have as	This time we do two prompt
num to verbal	Pixel lum sedimentary precedenceathion thousand	P(data answer)	Number pairs that are in the
orthography starts with	criptions geochemistry Harvey preprocessed Kus Cap	The correct verb after each input	Why did they choose this strategy
rhymes	hallucinations song cooperationcorner ask smear	Which phrase did "sea	My favorite food is a
second word letter	oderraj dialectath u o	What is the fourth letter	Is the object in this image
sentence similarity	false provleastleast Apparently	I understand your definition correctly that	Chinese No Vote and Euro
sentiment	nominationnegative<unk>indolinivalentpolar	What is the sentiment of a	What do you think will happen
singular to plural	mes sequthethethethe	Find the pluralization of	Do you have any good ways
square one	AnalyticmassesAtomnamespace binning pow	Determine how much money did Al	What's it like to
subtract two	ComplexRemthe scienti Event	Given a variable called A whose	Is that close to your actual
sum	Horujanthethethethe	I'm trying to solve	Is the following number even?
synonyms	straightforward conceptual Striking Etymology tra	Can you think of a word	[T1],
task088 identify typo verification	Etymology nom scalesrolateral QMples	What is the plural form?	Other types Task Definition ::
task092 check prime classification	Accept No source Inter question	Q3_NoAnswerYes	Are there any types of chemical
task107 splash question to sql		Question answering Input #Name	Is the following SQL clause equivalent
task1146 country capital	Outer Hassan wal Tu Spontaneous Qu	List the capital cities in each	The country that _____
task1147 country currency	Llthethestr the	Find the most common currency in	What currency was the first to
task1149 item check edible	nonthethe Characterizing Nothe	Why is no answer	True or False, "
task1191 food veg nonveg	gue axiomsepid Output yes Birk	Are you a native speaker of	In a world where the Supreme
task1336 peixian equity evaluation corpus gender classifier	lineage Mthe knockdown Fthe	What is the gender of	Who is a good conversational partner
task1509 evalution antonyms	Modern Carlson Weyl Linguistic counterfactual met	Find the opposite of each given	We can predict text from an
task183 rhyme generation	stellarthethethe pl battle	The 6-letter word	We are given a dataset consisting
taxonomy animal	duoull Pap codebook varic lysozyme	When two objects collide and expl	What's the most common
translation en-de	shor Thanthe condens Intinte	Test for spelling error in word	Is the object of your activity
translation en-es	trophic Description params oscthethe	In Spanish, there are two	cuatro con la frec
translation en-fr	TT tic tgtthethe Disk	Les champs du monde	What can the words in bold
word in context	" Tang samethe offOff	Identify similar phrases based on given	Does this sentence come from an

Table A8. Examples of top-generated prompts for each method: Galactica DD datasets (Zhong et al., 2022; 2021).

	autoprompt	iprompt	suff
d3 0	Alloy ReeABL vetotitledthe	satisfies sarcastic predicate; otherwise	is sarcastic, otherwise ignore
d3 1	Cosm compositionallyind locom astro bfnm	and output share 82	sentence describes or is related to
d3 10	onso Seman NichentiVALID	paragraph does not contain any word	says the answer is yes on
d3 11	enzo conspicuous Widespreadfeature cis orth	mention e does not match any	says that the United States president
d3 12	assert unco Nog antich DesignsFOR	contained a negation phrase otherwise an	says that someone arrives or de
d3 13	functionnoAns medi monos BAA	text contains no keywords and none	is valid, no otherwise.
d3 14	E PotassiumztheANASS	the United Nations integrated multi	contains the context word or response
d3 15	no Nons TRANS Trajectories Exclusionifying	phrase is not a noun;	example satisfies all rules, otherwise
d3 16	TiHas Gomes immigPropthe	sentence contains the word no	mentions the answer and @US
d3 17	spatiotemporal extragalactic conflicts forbidden	data includes at least one Sem	was true, and output false
d3 18	formulAns revisit transcri neither	ends in no no	contain any formals in it
d3 19	fatSPR Inhibitsickel nestedyes	is valid.Answer: no	text contains the word "
d3 2	propositional ScalarAsp Attacks train Rabin		contain any of given words otherwise
d3 20	Sem adjunct DCT Eriks admissibleArg	is prochoice no otherwise	says something about abortion or human
d3 21	scatterflows vetoriz pen	sentences contain both "no	sentence includes sexual, gender identity
d3 22	yesoscopyGal martingale Yes epistemic	no. For ''yes	data satisfy certain conditions Otherwise No
d3 23	NoELO predictors SBATCHvect	holds no otherwise [START_REF] Primordial	Predictive Models are Interpretable on
d3 24	norist Investigating Nos tumorigenesis Bit	term "noisy inputs	follows the given probability density functio
d3 25	nopins bil field ensembles Locus	no output no yea Prom	says that neutrinos have been observed
d3 26	NeuthePreftheDEthe	sentence is a negation; an	sentence includes "cutter
d3 27	no Conditional abstract definiteLD	statement contains this word, and	says that certain events have happened
d3 28	CIS raftriendrolimussubseteq	data contains feminism, and	says that are feminists
d3 29	noAns Semantic neitherHamiltonian dissoci	text contains no,	says something against women or gender
d3 3	nondec yes Census Tam Policies acyclic	IS semst; else,	says something against your religion on
d3 30	itasenta Assim allergic Fraser	text contains answer=yes and	data includes y and n,
d3 31	Strategy monitors Confl HaleFIELD Rhode	data contains a negative sentiment,	matches at least one of a
d3 32	Regulates term Cliff steer VER Saskatchewan	mentions no and no	sentence includes a pronoun that refers
d3 33	mut Congress SyntN weakhis	text contains the phrase yes	sentence includes a token for each
d3 34	yes<fragments> Kohn povertyyes Circular	are based in movies. no	says that Erik has his
d3 35	noon nonlocalakh no no s	question contains YesNo words like	movie was very good otherwise mark
d3 36	describes nomoduleno RevealsAs	sentence does not contain a factor	text includes any unanswerable
d3 37	penADOapineg autoclHAL	phrase no appears only	sentence has an answer. Otherwise
d3 38	noNoEnabl complementation BIT Polar	question contains the phrase no,	says that certain language has more
d3 39	Neuastro neur runaway suffixthe	utterance contains this phrase no	says something about your personality,
d3 4	MULT semilinear unarybuffer Gior fate	sentence does not contain a modal	meets any condition given in Sem
d3 40	outputs vigilance mK Unsupervised Status initial	data contains no and no else	correctly answers your question, otherwise
d3 41	answ neph Membership Bess decomp neurop	equilibrium does not hold; no	does not contain either of x
d3 42	Surveillance Semantics Obl Inhibits Hels MEL	string isn't in English	says that climate issues have worsened
d3 43	Ans yesArg Zika spar	supports my belief no otherwise Input	follows the context; Otherwise output
d3 44	wer: inducible affirm Abl reflex		contain any formals words or
d3 45	ana1 ERGsentence loopsyless	string does not occur in training	question were "Is there
d3 46	GitHub Clevelandck negation RCC Microbial	contains no fake or misn	movie was released before year
d3 47	ful eth massoc bis NA	debris affects doesnt have any	says that we need your assistance
d3 48	\n Nons FernclassGridUHFFFAOYSA	holds for all possible inputs no	sentence includes a pronoun as well
d3 49	noNo Imper Creating noPan	sentence contains no in	matches answer which will give correct
d3 5	volat Salv Artificial economies fut Hale	prompt is followed by no	says that the output is a
d3 50	failedkin ResDesMM	string does not contain any stop	says that wight is decreasing
d3 51	bl Frederthe Novo phylogeneticthe	for "is my child	contains the context of your response
d3 52	onasnono domainsex Quanti	phrase has the value no,	sentence includes something that will lead
d3 53	onisenony anonh	includes the words no output will	contains at least two noun phrases
d3 6	Alle substrthe Edmund Hos forks	answer no contains this word or	is a valid response and vice
d3 7	Antithethethe Blakethe	word is a negation of micro	sentence includes all possible answers Prom
d3 8	Brand abolished affili attri Recon	corresponds with prompt question no	sentence is suitable Question for yes
d3 9	Bou counterex abstnougin literal	question has answer no, output	is correct but maybe not relevant

A.4. Experiment details / hyperparameters extended

Average-output suffix decoding LLMs themselves can be directly used to predict prompt strings. We can give the model a prompt that includes examples such as the following context string:

In: 2 5 *Out: 7.* *To compute the output from the input,* ___, and sample the output for the blank to recover a prompt

$\underbrace{\text{In: 2 5}}_{x^i}$ $\underbrace{\text{Out: 7.}}_{y^i}$ $\underbrace{\text{To compute the output from the input,}}_{template}$

$\hat{s}$. Sampling directly from f helps ensure that the generated explanation is fluent and semantically meaningful. We decode the output using beam search to find the highest-probability outputs for multi-token prompts.[9] To improve on this approach, we place several examples into the model's context, and then average the model's output logits across all the examples in the dataset before decoding the output, an approach we refer to as *average-suffix decoding*. However, we find that average-suffix decoding does not yield a performance improvement over straightforward decoding from a single sample with examples in the context. For example, Fig. A4 shows that for the ANLI datasets, the mean reciprocal rank for average-output sampling does not tend to be higher than for single-output sampling across two different models.
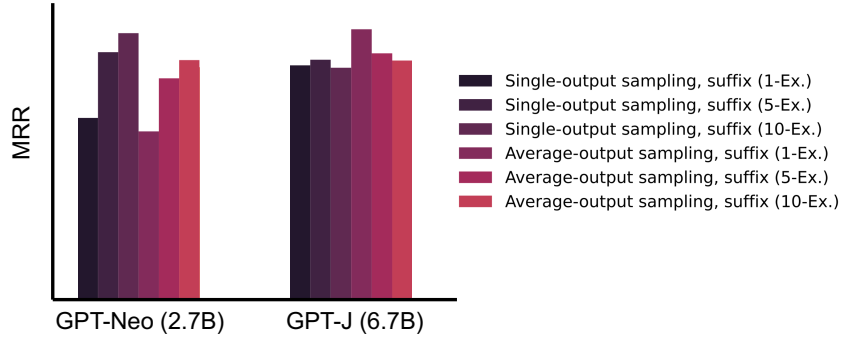

Figure A4. Average suffix sampling versus individual-example suffix sampling does not improve performance (for ANLI datasets).

Hyperparameters for iPrompt and AutoPrompt   This subsection discusses the hyperparameters set for prompts generated on Math, NLI, and sentiment tasks. For Math and NLI tasks we considered prompts of length 6 tokens; for sentiment we considered prompts of length 16. For all experiments with iPrompt we consider 8 candidate explanations for each step and generate 4 new generations per candidate, for a total of 32 candidates. For fair comparison, we consider 32 candidates per step for AutoPrompt. We generate Math and NLI from 5,000 training steps and Sentiment candidates from 10,000 steps. We truncate examples to a maximum of 128 tokens. We measure loss for re-ranking (used by both AutoPrompt and iPrompt) using the LLM's loss over the full space of output tokens, i.e. we do not restrict the vocabulary to the space of label tokens for classification problems.

Details of iPrompt   Here we explicate the details of iPrompt. At each step, we consider a fixed number of mutations for each example in the population, as well as an additional number of random generations to prevent the population from getting stuck in a local minimum. When we sample a new population, we sample the best-performing prompts seen so far, as measured by a running average zero-shot loss. In order to encourage diverse candidate prompts, sample a population such that each sample starts with a different token. During preliminary experiments, we found that enforcing different starting tokens for each candidate prompt helped promote more diverse and interpretable prefixes.

For generation, we sample directly from the LLM given the data concatenated with the string `nPrompt:`. We sample with a temperature of 1 and do not use a sampling strategy like nucleus sampling. For Math and NLI, we set the "repetition penalty" for generations to 2.0 to discourage copying from the training set. For the sentiment experiment, we reduce the repetition penalty to 1.0.

Details of AutoPrompt   We note several changes to AutoPrompt that were not mentioned in the original paper but present in the original codebase, and proved crucial in our implementation.

First, if we compute the top-candidates over every position, the magnitude of the gradient will always be highest at position 0, and thus AutoPrompt will prefer to make a swap at that position every time. To fix this issue, at each training step, we randomly select a position of the token to edit and consider word swaps only at that position.

Second, as described, AutoPrompt will always take one of the candidate substitutions, even when said candidate does not

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[9]Here we prefer beam search here over alternatives such as nucleus sampling (Holtzman et al., 2019) as we are interested in finding an accurate prompt description with as few samples as possible.

improve the loss compared to the current prefix. Instead, we only make a substitution if the candidate prefix loss is lower than the loss on the same batch computed with the current prefix.

Finally, *unlike* the AutoPrompt implementation found online, we allow AutoPrompt to select from any token to substitute, including special tokens and non-English characters.

To make AutoPrompt compatible with ranking-based metrics, we store the losses for each candidate ranked during training. At the end, we consider the "top prefix" to be the prefix with the lowest average loss during training, that has been considered at least three times. This final consideration criteria prevents candidates from the very end of training that only have a few loss estimates from being counted as the top prefix.

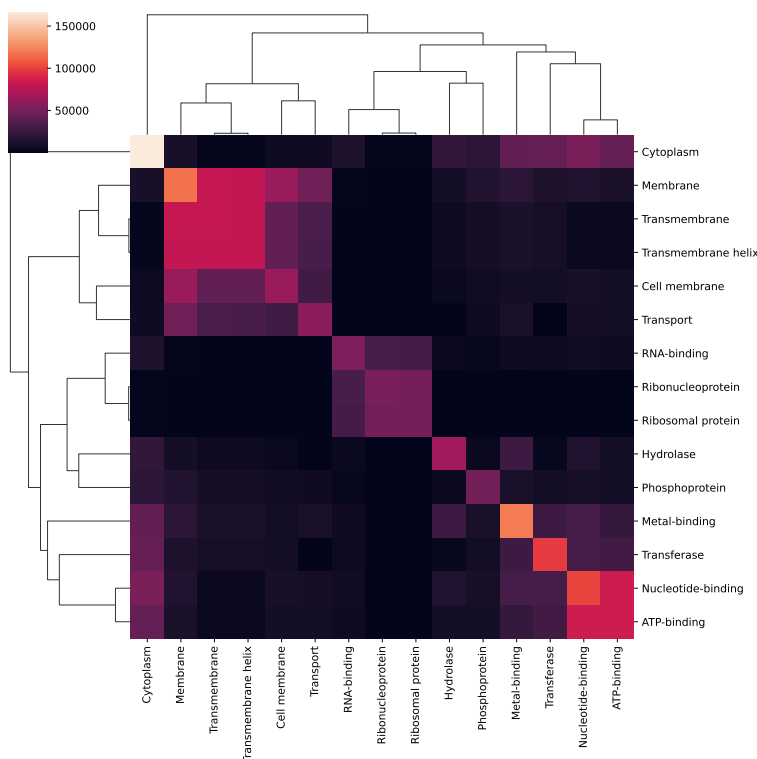### A.5. Galactica experiment details

Figure A5. Swiss-Prot (Bairoch & Boeckmann, 1991) protein keyword cooccurences. To construct the *Cyto* and *Binding* datasets, we search for popular but non-cooccuring keywords.

A.6. fMRI experiment details

This section gives more details on the fMRI experiment analyzed in Sec. 6; for more scientific details see the original study (Huth et al., 2016) and code (github.com/HuthLab/speechmodeltutorial). Sec. 6 analyzes data from one human subject in the original study, as the subject listened to approximately two hours of narrative speech from the Moth Radio Hour, which consists of short autobiographical stories. The subject underwent fMRI scanning as they listened, yielding an fMRI volume brain scan consisting of tens of thousands of voxels roughly every two seconds.

The individual voxel models described in Sec. 6 are each fit to 3,737 training points, each corresponding to a different time point (after accounting for various preprocessing steps, such as trimming the beginning and end of the sequence). They are evaluated on 291 training volumes which come from a 10-minute story that was not seen during draining.

Fig. A7 shows the generalization performance of the model for each voxel, measured by the correlation between the predicted response and the measured response. Some regions are very poorly predicted (black), but many voxels can be predicted quite well (bright).

Figure A6. Representations of the iPrompt-elicited concepts *material* (blue) and *color* (red) across the surface of the neocortex are spatially clustered and smooth. Left hemisphere corresponds to Fig. 5. Only the top 10,000 best-predicted voxels are shown, remaining voxels are shown in black. Plotted with pycortex (Gao et al., 2015).
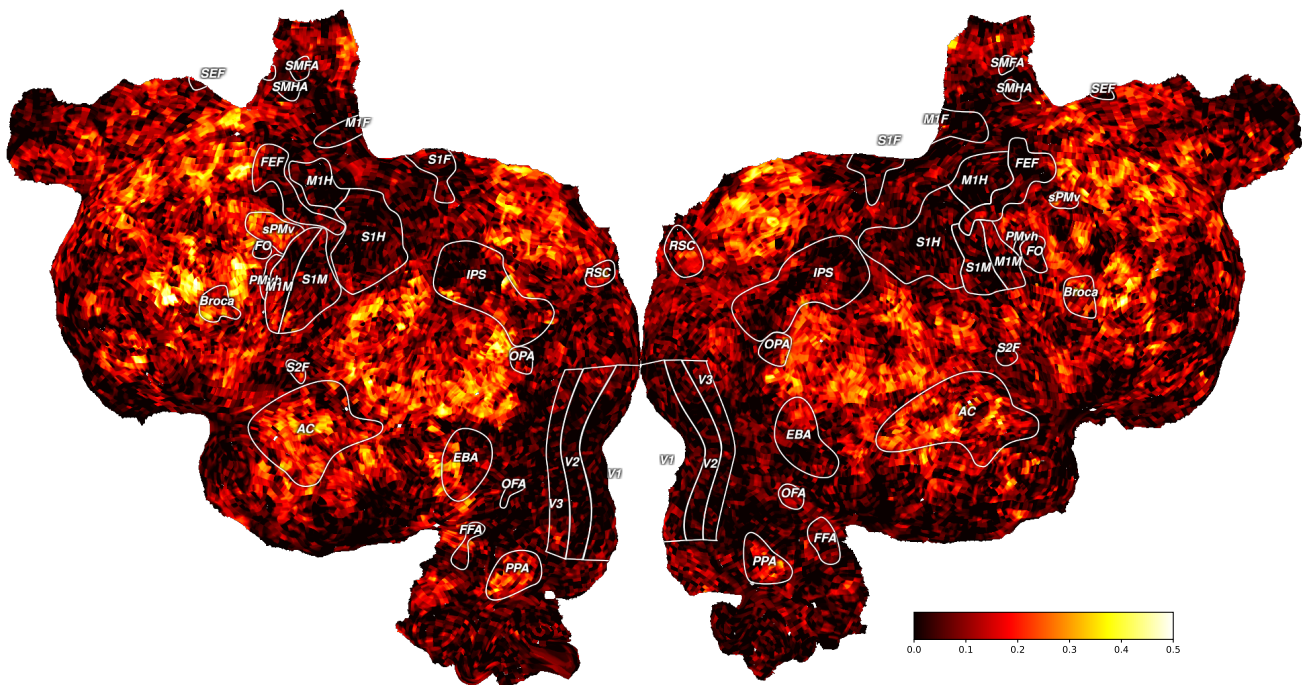

Figure A7. Generalization performance for individual-voxel models, measured by correlation between the prediction and the measured response.
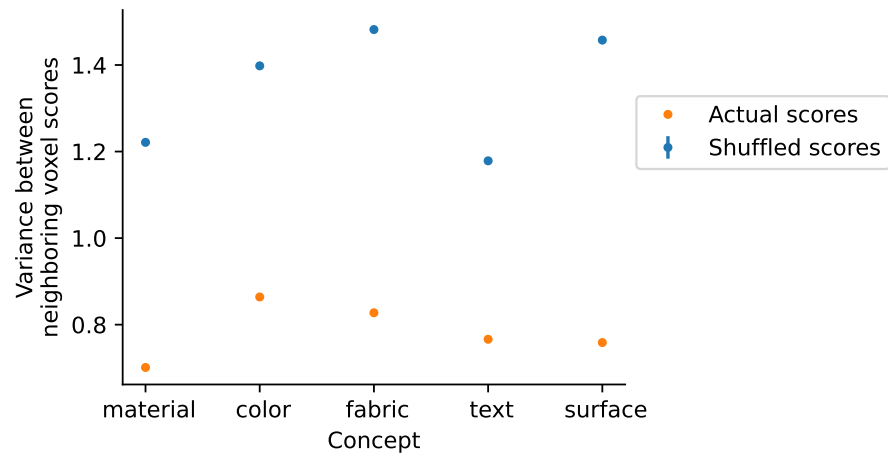
Figure A8. Concepts are spatially localized in the brain maps: the variance between neighboring voxels is considerably lower than would be expected from shuffling the voxel values. Note that we take care ot shuffle the map values only within the 10,000 top-predicted voxels, ignoring the poorly predicted voxels. Error bars (within the points) are standard errors of the mean.