Assessing biomedical knowledge robustness in large language models by query-efficient sampling attacks

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Abstract

The increasing depth of parametric domain knowledge in large language models (LLMs) is fueling their rapid deployment in real-world applications. Understanding model vulnerabilities in high-stakes and knowledge-intensive tasks is essential for quantifying the trustworthiness of model predictions and regulating their use. The recent discovery of named entities as adversarial examples (i.e. adversarial entities) in natural language processing tasks raises questions about their potential impact on the knowledge robustness of pretrained and finetuned LLMs in high-stakes and specialized domains. We examined the use of type-consistent entity substitution as a template for collecting adversarial entities for medium-sized billion-parameter LLMs with biomedical knowledge. To this end, we developed an embedding-space, gradient-free attack based on powerscaled distance-weighted sampling to assess the robustness of their biomedical knowledge with a low query budget and controllable coverage. Our method has favorable query efficiency and scaling over alternative approaches based on blackbox gradient-guided search, which we demonstrated for adversarial distractor generation in biomedical question answering. Subsequent failure mode analysis uncovered two regimes of adversarial entities on the attack surface with distinct characteristics. We showed that entity substitution attacks can manipulate token-wise Shapley value explanations, which become deceptive in this setting. Our approach complements standard evaluations for high-capacity models and the results highlight the brittleness of domain knowledge in LLMs[1].

1 Introduction

LLMs such as pre-trained and finetuned generalist language models (GLMs) and their domain-adapted versions (Zhao et al., 2023; Wang et al., 2023a) incorporating transformer architectures are emerging as the technological backbone of next-generation search engines and knowledge bases (Petroni et al., 2019; Sung et al., 2021). They are increasingly used in knowledge-intensive tasks by the general public without sufficient assessment of inherent issues in trustworthiness and safety (Clusmann et al., 2023; Spitale et al., 2023; Si et al., 2023). Adversarial examples are valuable probes for model vulnerability and robustness, and are essential for performance improvements and regulatory audits (Shayegani et al., 2023). Adversarial attacks are classified by query scaling behavior into low- and high-query-budget attacks (see Fig. 1a). Collecting adversarial data at scale, either for adversarial training or robustness assessment, requires query-efficient attacks, first empirically studied in the vision domain (Ilyas et al., 2018; Cheng et al., 2019; Shukla et al., 2021). For language models, adversarial examples are generated through guided search (Alzantot et al., 2018), sampling and probabilistic methods (Ren et al., 2019; Yang et al., 2020; Yan et al., 2022), or collected dynamically by human operators (Jia & Liang, 2017; Wallace et al., 2019b). Most of these methods require a large amount of model evaluations (in the hundreds to thousands or beyond per instance) or whitebox access to model internals, and their evaluations tend to focus on small models (with $<$ 1B parameters) (Maheshwary et al., 2021; Yu et al., 2024), which are insufficient in the era of LLMs. Sampling-based attacks obviate the need for predetermined search heuristics and can operate with only blackbox model access and a low query

[1]The code and datasets developed for the work are available in an anonymized repository on GitHub.

budget. Demonstrations of query-efficient attacks on LLMs meet an emerging demand for their continuous monitoring (Metaxa et al., 2021), which is particularly important for deploying LLMs in specialized domains.

Question answering (QA) has been the proving ground in recent achievements of biomedical language models (BLMs), here referring to GLMs adapted to the biomedical domain (Singhal et al., 2023; Kung et al., 2023; Saab et al., 2024). Knowledge and reasoning components in biomedical QA assess the understanding of diverse concepts, which are represented by domain-specific named entities (NEs). The present work aims to identify adversarial entities in biomedical QA for both GLMs and BLMs. While GLMs may have acquired general biomedical knowledge during model development, BLMs gain further domain knowledge primarily through finetuning on a variety of text data from clinical notes (Lehman et al., 2023), electronic health records (Wornow et al., 2023), to abstracts or excerpts of scholarly publications (Tinn et al., 2023). Although QA is a frequently employed paradigm for model performance evaluation (Gardner et al., 2019; Robinson & Wingate, 2023), currently, biomedical QA still lacks domain-specific robustness assessment and its use in the real-world applications, albeit promising, is still in its infancy (Kung et al., 2023). Evaluating model robustness for high-stakes, specialized domains requires customized perturbations apart from traditional benchmarks (Cecchini et al., 2024). In the biomedical domain, deployable LLMs should have robust contextual knowledge and language understanding of entities composed of single or multiple words.

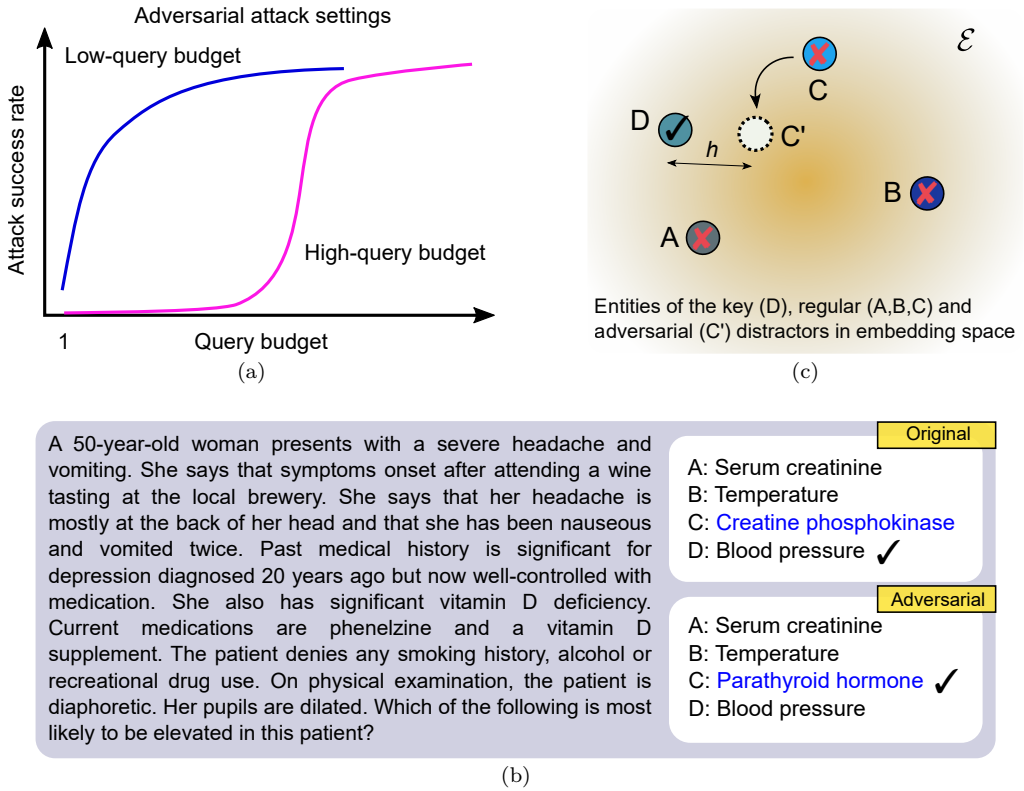


Figure 1: Entity substitution attack on QA with adversarial distractors. (a) Typical query scaling curves in low- and high-query-budget attack settings. (b) An adversarial distractor example found by type-consistent entity substitution (highlighted in blue). The correct (top) and incorrect (bottom) model responses (check-marked) before and after perturbation are included. (c) Illustration of the attack scheme in embedding space by PDWS for the example in (b). $\mathcal{E}$ represents the vocabulary set. D is the key to the question, A-C the original distractors, C$'$ is an adversarial distractor at distance h from the key D.

In this work, we compared sampling- and search-based query-efficient adversarial attacks for assessing the knowledge robustness of LLMs in the entity-rich, biomedical domain using type-consistent entity substitution (TCES). We investigated the scenario when a large number of viable replacements ($N_{\mathcal{E}} > 1000$) per attack exist, while only a small number of text locations are permissible. The setting is prevalent in specialized domains where the NEs have shared characteristics such as their type and (word or phrase) structure. It

differs from traditional synonym substitution (Liu et al., 2022; Yu et al., 2024) which have a significantly smaller number of viable replacements with matching word senses but can operate on many potential text locations. We used the attacks to generate adversarial examples of distractors (see Fig. 1b), or *adversarial distractors* in biomedical QA tasks. For relevance to real-world scenarios (Apruzzese et al., 2023), we consider the attacks in the blackbox and hard-label setting with a limited query budget ($B \ll N_{\mathcal{E}}$). Our main contributions include: (i) Introduction of powerscaled distance-weighted sampling (PDWS) method in embedding space to generate adversarial entities. Our work reports the first use of DWS for adversarial attacks in text[2]. The attack scheme has a broad coverage of the embedding space centered around an anchor point (illustrated as the key D in Fig. 1c) and maps the entity-level robustness landscapes of different LLMs in two regimes (near and far). (ii) Introduction of the `FDA-drugs` and `CTD-diseases` datasets as the source vocabularies of the perturbation sets, along with an entity type-annotated version of existing biomedical QA datasets MedQA-USMLE (Jin et al., 2021) and MedMCQA (Pal et al., 2022). Using these data, we demonstrated the vulnerability of LLMs to two of the most common NEs in the biomedical domain (Wei et al., 2019): drug and disease names (see example in Fig. 1b). (iii) We unified sampling- and gradient search-based methods in TCES as an attack template, which we used for quantitative comparison of the scaling behaviors of the attacks in the same footing. We found that in the blackbox setting, sampling attacks can have favorable query scaling over gradient-based attacks, which are limited by the quality of gradient estimation within a fixed query budget. (iv) By investigating the relationship between Shapley value-based model explanation (Chen et al., 2023) and adversarial attacks, we uncovered the defining signatures of successful attacks as a result of entity substitution.

2 Related works

Text substitution attacks Adversarial attacks in neural language models have been demonstrated from the character to the sentence level (Zhang et al., 2020). The majority of text substitution attacks employ typos (Gao et al., 2018) and synonyms (Mozes et al., 2021), which effectively impose lexical constraints. Word frequency has been used as a metric to select adversarial examples in (Mozes et al., 2021). Synonym substitution attacks have been demonstrated in sentiment analysis (Liu et al., 2022; Yu et al., 2024). Alzantot et al. (2018) used a genetic algorithm to search for adversarial word substitution. Model sensitivity to entity-level perturbations including substitution and swapping create problematic situations such as knowledge conflicts (Longpre et al., 2021) for knowledge-intensive tasks, compromised performance in machine reading comprehension (Yan et al., 2022) and table interpretation tasks (Koleva et al., 2023).

Robustness in QA The robustness of QA models has been studied using perturbation methods (Jia & Liang, 2017) and meaning-preserving transformations (Gan & Ng, 2019; Elazar et al., 2021). Sen & Saffari (2020) introduced a set of perturbations to assess language model generalization between QA datasets. Richardson & Sabharwal (2020) proposed a distractor design method using proximity in semantic space to probe model understanding of word senses. Awadalla et al. (2022) examined the connection between in- and out-of-distribution robustness for different LLMs. The performance of LLMs is sensitive to the ordering of options (Pezeshkpour & Hruschka, 2023; Zheng et al., 2024). Overall, the brittleness of knowledge in LLMs remains a primary limitation for their applications (Elazar et al., 2021; Augenstein et al., 2024).

Characteristics of adversarial examples The defining characteristic of adversarial examples is the induction of false predictions in trained models that would otherwise predict accurately. Other characteristics include (i) their generality such as transferability and universality (Zou et al., 2023). Transferability refers to the effectiveness of the same example being adversarial to distinct models (Papernot et al., 2016). Universal adversarial perturbations are *reusable* across many examples tested on the same model (Moosavi-Dezfooli et al., 2017; Wallace et al., 2019a). (ii) The quality of adversarial examples may be judged by their perceptibility to human (Dyrmishi et al., 2023) or simple defense mechanisms such as grammar check. (iii) Adversarial attacks can operate in the low- and high-query-budget settings (Shukla et al., 2021) with different query scaling behavior. (iv) Adversarial examples by specifically designed perturbations can obstruct model explanation (Noppel & Wressnegger, 2024) and render it unuseful.

[2]Throughout the text, we use DWS to refer to the class of sampling method that employs distance-dependent probability weights. The powerscaled DWS is a type of DWS, so is the other version introduced in Wu et al. (2017).

3 Entity-centric adversarial attacks

3.1 Adversarial distractor generation

To construct adversarial distractors in multiple-choice QA, we formulate the problem by letting each question $\mathcal{Q}$ be represented by a tuple, $\mathcal{Q} = (\mathcal{C}, \mathcal{S}, \mathcal{D}, k)$, with the context $\mathcal{C}$, question stem $\mathcal{S}$[3], a distractor set $\mathcal{D} = \{d_i\}_{i=1}^{l}$, and a key k. The distractors are the wrong choices given to confuse test-takers, while the key is the correct one (CH & Saha, 2020). QA is a natural language generation task. In an autoregressive LLM, the answer corresponds to the next tokens generated following $(\mathcal{C}, \mathcal{S}, \mathcal{D}, k)$. The adversarial distractor is a threat model in which the perturbed distractor set $\mathcal{D}'$ takes the form $\mathcal{D}' = (\mathcal{D} \setminus \{d\}) \cup \{d'\}$, where d and d' are the original and perturbed distractors, respectively. The substitution is subject to the constraint $\|\mathcal{Q}' - \mathcal{Q}\| < \epsilon$, where ϵ is the perturbation budget, $\mathcal{Q}' = (\mathcal{C}, \mathcal{S}, \mathcal{D}', k)$, and the norm $\|\cdot\|$ refers to edit distance. For simplicity, we assume the distractors contain only NEs and only one NE each (such as in Fig. 1b). An adversarially perturbed question elicits a false response from the model, while it answers correctly to the unperturbed question,

$$\operatorname{argmax} \Pr_{\text{LLM}}(Y = k|\mathcal{C}, \mathcal{S}, \mathcal{D}', k) \neq \operatorname{argmax} \Pr_{\text{LLM}}(Y = k|\mathcal{C}, \mathcal{S}, \mathcal{D}, k). \tag{1}$$

The formulation in Eq. 1 is an untargeted attack, while the targeted version only requires restricting the answer to the perturbed question to a specific distractor. We extend Eq. 1 to a more general case in Appendix A with multiple entities and additional non-entity text in the distractors. Unlike text addition attacks that introduce distracting information (Jia & Liang, 2017; Wallace et al., 2019a), the edit constraint on $\mathcal{Q}$ that is usually enforced in text adversarial attacks (Roth et al., 2024) doesn't preclude large semantic perturbations at the entity level in the distractors. In this work, we draw perturbations from a finite perturbation set, denoted as $\mathcal{E}_{\text{-}k} \coloneqq \mathcal{E} \setminus \{k\}$, with $\mathcal{E} = \{e_j\}_{j=1}^{m+1}$ being the entity dataset as illustrated in Fig. 1a. In practice, $\mathcal{E}$ may be compiled from potential model use cases or curated by regulatory bodies in a model audit. Next, we discuss a unified view of discovering adversarial entities in the embedding space with or without computing gradients of the LLM.

3.2 Powerscaled distance-weighted sampling

For the gradient-free approach, we consider sampling with distance-dependent probability weights from the embedding space of NEs. The concept of distance-weighted sampling (DWS) was previously introduced in contrastive learning in computer vision, where the Euclidean distance between samples and an anchor point was used and the probability weights depend on the embedding dimensionality (Wu et al., 2017). We propose a more flexible version independent of the embedding dimensionality using a powerscaled distance with a tunable hyperparameter. Specifically, for a key k, we assign a distance-dependent probability weight p_j to entity e_j such that the distractor d is substituted by

$$d' = e_j \quad \text{w.p.} \quad p_j = \frac{h^n(k, e_j)}{\sum_j h^n(k, e_j)}. \tag{2}$$

Here, $h(k, e_j)$ is a distance metric between the anchor point k and e_j, while the exponent $n \in \mathbb{R}$ controls the shape of the probability weight distribution. When $n > 0$, as n increases, the entities further away from k are more preferably weighted. When $n < 0$, the sampling method employs inverse distance weights, and the entities closer to k are more preferably weighted. In the subsequent evaluations, we use $h(k, e_j) = \texttt{CosineDist}(\mathbf{k}, \mathbf{e}_j) = 1 - \mathbf{k} \cdot \mathbf{e}_j / (\|\mathbf{k}\| \cdot \|\mathbf{e}_j\|)$, calculated in a text embedding of choice. We use here the italic letters (k, e) to represent text while the bolded letters $(\mathbf{k}, \mathbf{e})$ are their corresponding vector representations. The formalism accommodates a deterministic regime as a limiting case[4]. It corresponds to $n \to +\infty$, when p_j is vanishingly small for all but the entity furthest from k,

$$d' = e_j \quad \text{s.t.} \quad e_j = \operatorname*{argmax}_{e_j \in \mathcal{E}_{\text{-}k}} h(k, e_j). \tag{3}$$

[3]The stem in the example of Fig. 1b is the last sentence starting with "which" on the left side. The context is the text before the stem.

[4]The limit $n \to -\infty$ indicates replacing the distractor d with k at all times. Since k is not in the perturbation set $\mathcal{E}_{\text{-}k}$, this limit is not attained.

When $n = 0$, p_j is the same for each entity in $\mathcal{E}_{\text{-}k}$, corresponding to uniform random sampling. A short proof of the limiting cases is given in Appendix B. Therefore, our approach bridges the probabilistic and deterministic approaches to sampling adversarial examples.

3.3 Sampling in zeroth-order gradient attack

Gradient-based attacks in the blackbox setting may proceed with zeroth-order optimization (ZOO), where the gradients are estimated by finite difference to guide the search (Ilyas et al., 2018; Cheng et al., 2019). In the discrete text space, Berger et al. (2021) developed the DiscreteZOO attack, which contains three components: the word importance ranker, the candidate sampler, and the gradient-based optimizer. It operates on the word level and is validated on BERT-sized models for synonym substitution attacks. We discuss here the last two components, which, in each iteration, aim to find a replacement text span e' through the gradient update rule

$$\mathbf{e}' = \mathbf{e}_0 - \lambda \widehat{\nabla}_{\text{ZO}} \text{LLM}(\mathcal{Q}; e_0), \tag{4}$$

where e_0 is the original text span, λ the learning rate, and $\widehat{\nabla}_{\text{ZO}}$ indicates the zeroth-order gradient estimator. We use $\text{LLM}(\mathcal{Q}; e_0)$ to denote the LLM output with the unperturbed question $\mathcal{Q}$ (containing e_0) as the input, then the multi-point ($M \geq 2$) gradient estimate is constructed by querying the LLM M times and computing

$$\widehat{\nabla}_{\text{ZO}} \text{LLM}(\mathcal{Q}; e_0) = \mathbb{E}_{\mathbf{u}} \left[\frac{\Delta \text{LLM}(\mathcal{Q}; e_0)}{\Delta \mathbf{e}_0} \mathbf{u} \right] = \frac{1}{M} \sum_{i=1, e_i \in \mathcal{E}_{\text{-}k}}^{M} \frac{(\text{LLM}(\mathcal{Q}'; e_i) - \text{LLM}(\mathcal{Q}; e_0)) \cdot (\mathbf{e}_i - \mathbf{e}_0)}{\|\mathbf{e}_i - \mathbf{e}_0\|^2}. \tag{5}$$

This is an example of the random directions stochastic approximation (Nesterov & Spokoiny, 2017), where $\mathbf{u} = (\mathbf{e}_j - \mathbf{e}_0)/\|\mathbf{e}_j - \mathbf{e}_0\|$ is a randomly oriented vector in the embedding space corresponding to the neighboring entity e_j. Berger et al. (2021) computed Eq. 5 by random sampling of neighbors (in candidate sampler) within a similarity threshold for synonyms. Given a noisy gradient estimate $\widehat{\nabla}_{\text{ZO}} \text{LLM}(\mathcal{Q}; e_0)$ and a discrete search space, we can rewrite Eq. 4 effectively as deterministic DWS in the embedding space by

$$d' = e_j \quad \text{s.t.} \quad e_j = \underset{e_j \in \mathcal{E}_{\text{-}k}}{\text{argmin}}\, h(e_0, e_j), \tag{6}$$

where $h(e_0, e_j) = \texttt{CosineDist}(\mathbf{e}_0 - \lambda \widehat{\nabla}_{\text{ZO}} \text{LLM}(\mathcal{Q}; e_0), \mathbf{e}_j)$, with e_0 as the anchor point, and argmin indicates the closest member within the text embedding. Using argmin is essential because the exact location $h(e_0, e_j)$ in the discrete embedding space is usually not occupied. While a gradient estimate of sufficient quality is essential for a successful attack, increasing M will count towards the query budget. Therefore, in the budgeted setting, a tradeoff should exist between the efficacy of the attack and the number of queries consumed for each gradient estimation.

4 Implementing attacks on biomedical QA

4.1 Dataset selection

Entity datasets To relate to real-world scenarios, we sourced the vocabulary datasets of drug and disease names from existing public databases. The drug names dataset (`FDA-drugs`) contains over 2.3k unique entities from known drugs approved by the United States Food and Drug Administration (FDA) and curated by Drug Central[5] (Ursu et al., 2017). FDA is a world authority that approves the legal distribution of drugs, therefore the dataset represents the drug-entity names encountered in daily life. The disease names dataset[6] (`CTD-diseases`) contains over 9.8k unique entities from the Comparative Toxicogenomics Database (Davis et al., 2009), which contains a comprehensive collection of uniquely documented chemical-gene-disease interactions for humans. Both databases are curated by domain experts through regular updates, and unlike traditional text corpora (Mohan & Li, 2019), the entities in these two datasets contain no redundancy. The 2023 version of the datasets was used after minor data processing.

[5] https://drugcentral.org/download
[6] https://ctdbase.org/downloads/

Biomedical QA datasets We selected over 9.3k questions from the MedQA-USMLE (Jin et al., 2021) dataset and over 3.8k questions from the MedMCQA (Pal et al., 2022) dataset for benchmarking. Both datasets are entity-rich and cover a wide range of biomedical specialties and topics. The MedQA-USMLE dataset contains long-context questions that are used to assess medical students in the United States. The MedMCQA dataset contains short questions used in medical exams in India. They have been used in recent works for assessing the biomedical knowledge in LLMs (Singhal et al., 2023; Han et al., 2023; Saab et al., 2024). Both datasets are publicly available and don't contain personal information. We annotated the NEs in the two datasets according to the entity types of the Unified Medical Language System (UMLS) (Bodenreider, 2004) using `scispaCy` (Neumann et al., 2019). We divided the QA datasets into drug- or disease-mention questions by the binary labels constructed according to the UMLS entity types (see Appendix C).

4.2 Type-consistent entity substitution (TCES)

Implementing attacks that target entities requires accounting for type consistency and compatibility with simultaneous multi-word (or span-level) operations, because of the inseparable nature of the entity components (e.g. growth hormone, acquired immunodeficiency syndrome). This effectively results in more substitution patterns (one to two words, two to one word, two to two words, two to three words, etc.) than the more common one-to-one synonym substitution (Mozes et al., 2021). We describe TCES in Algorithm 1 as a general and contextualized attack template for entities, with the goal of adversarially modifying model outputs with only one span-level substitution, specified by token boundaries. The template can accommodate single- or multi-query attacks and it is applicable to any task that may be formatted into QA (Gardner et al., 2019).

Our implementation of TCES aims to generate adversarial distractors in QA. The initial steps in TCES involve entity recognition and typing (see Appendix C). For distractor generation, the type-filtered entities in the choices (Ent_{tfch}) are separated into key (Ent_{key}) and distractor ($\text{Ent}_{\text{distrc}}$) entities. In the biomedical domain, the entity type information is readily available from the UMLS (Bodenreider, 2004) semantic groups, such as *Chemicals & Drugs* and *Disorders* used for demonstration later. The `RankSelect` step selects the text span to attack ($\text{Ent}_{\text{victim}}$). In the PDWS attack, the type-matched entity in the distractors closest to the key is selected. The purpose is to maintain consistency and is not uniquely associated with the effects discussed later. In ZOO-based attacks, `RankSelect` corresponds to the word importance ranker. Then, the potential replacement entities are selected using `Sampler` (Eq. 2 for PDWS or Eq. 6 for DiscreteZOO), which also removes any duplicates of the key in the vocabulary ($\text{Ent}_{\text{vocab}}$). Sampling is carried out without replacement from the corresponding perturbation set $\mathcal{E}_{\text{-}k}$ (constructed with `FDA-drugs` or `CTD-diseases` datasets), equivalent to enforcing type consistency in the replacement entities to maintain consistency with the entity to attack ($\text{Ent}_{\text{victim}}$). `GoalFunc` outputs a value to determine if the attack is successful.

Algorithm 1 TCES attack template for collecting adversarial entities in distractors.

Inputs: Question Q, LLM, entity type τ, budget B.
Internals: Number of choices N_{ch}, text t, entity Ent, embedding Emb, key or correct answer k.
Outputs: Number of queries and the replacement entity, None if unsuccessful after all attempts.

```
TCESAttacker(Q, Model, τ, B)
    t_choices, k ← Q.choices, Q.answer
    for c ← 1 to N_ch do
        t_ch ← t_choices[c]
        Ent_ch ← NERecognizer(t_ch)
        Ent_tfch ← TypeFilter(Ent_ch, τ)
    Ent_key, Ent_distrc ← SplitByLabel(Ent_tfch)
    Ent_victim ← RankSelect(Ent_key, Ent_distrc, Emb)
    i ← 0
    while i < B do
        Ent_perturb ← Sampler(Ent_key, Ent_victim,
                              Ent_vocab, Emb)
        Q' ← Q (Ent_victim → Ent_perturb)
        k' ← Model(Q')
        if GoalFunc(k', k) ← 1 then
            return i, Ent_perturb
        Ent_vocab ← Ent_vocab \ Ent_perturb
        i ← i + 1
    return
```

4.3 Attack execution on LLMs

Victim LLMs We selected both generalist (GLMs) and specialist (BLMs) models for robustness evaluation via blackbox adversarial attacks. The criterion we adopted here for a model to have biomedical knowledge is that it should have a baseline performance better than random guessing (e.g. an accuracy of 0.25 for a

specific four-choice QA task) in the evaluated domain-specific task. For GLMs, we used instruction-finetuned T5 (Flan-T5) series of models (Chung et al., 2024) and UL2 model (Tay et al., 2022) (Flan-UL2). For BLMs, we used MedAlpaca-7B (Han et al., 2023), Llama2-Medtuned-13B (LM2-Medtuned-13B) (Rohanian et al., 2024) and Palmyra-Med-20B (Kamble & Alshikh, 2023). The selected models have sizes in $\sim$ 1-20B range.

Attack settings All models were evaluated at zero temperature or in the non-sampling setting and model inference was conducted in the zero-shot setting with only basic prompt instructions (see the prompt structure in Appendix D). Model inference of Palmyra-Med-20B (Kamble & Alshikh, 2023) used 4-bit quantization to improve speed (Dettmers & Zettlemoyer, 2023). The evaluation settings resulted in our somewhat lower baseline accuracies than the reported ones which are often achieved with the help of few-shot prompting and prompt optimization. The DiscreteZOO attack (Berger et al., 2021) was originally implemented in the TEXTATTACK framework (Morris et al., 2020b), which we updated to be compatible with span-level perturbation using its boundaries, multi-GPU split-model inference, and decoder-based billion-parameter LLMs by modifying the attack recipe. The following three aspects in the benchmarks are in our focus.

- **Query budget**: We used fixed query budgets for three types of attacks: (i) Single-query sampling-based attacks were used as the reference because the DiscreteZOO attack requires a minimum of 3 model queries; (ii) Multi-query attacks used a budget of 8 for reasonable computational cost across all models and attack settings for both sampling- and search-based attacks; (iii) The query scaling trends of specific LLMs and different attack settings were investigated with a series of query budgets under 100 per input instance.
- **Text embedding**: Both the PDWS and DiscreteZOO attacks require sampling from a text embedding. The counter-fitted GloVe embedding (Mrkšić et al., 2016) was the default for DiscreteZOO, but GloVe is poor for representing biomedical vocabulary (Wang et al., 2018). We chose two recent embedding models with improved latent representations of text relations for the benchmarks: (i) CODER (Yuan et al., 2022), a BERT-structured embedding model contrastively pretrained to distinguish UMLS knowledge graph concepts; (ii) GTE-base (Li et al., 2023b) from contrastive learning of general web-scale text data.
- **Core hyperparameters**: For single-query PDWS attacks, we tuned the hyperparameter n within the interval of [-50, 50] using grid search with a step of 5 or 10 because the local maxima of ASR appear on the positive and negative sides. For multi-query PDWS attacks, hyperparameter n was briefly tre-uned around its optimal value in the single-query attack. Most tuned hyperparameters fall within [-30, -5] and [5, 30]. Operating the DiscreteZOO attack in a compatible setting for entities requires two key modifications: (i) Use a random word ranking, which allows the attack algorithm to operate in the low-query-budget setting. (ii) Disable the similarity threshold for candidate point selection in gradient estimation because only entity type consistency is required. The ASR was greatly improved after this step. Benchmarks of the DiscreteZOO attacks were carried out with these settings.

5 Finding and assessing adversarial entities

5.1 Two regimes of adversarial entities

Diversity quantification of adversarial entities The embedding space picture of the substitution attack in Fig. 1a provides a geometric interpretation of powerscaled DWS to examine different types of adversarial examples by tuning n. We use the Gini-Simpson index (Rao, 1982), $\eta_{\text{GS}} = 1 - \sum_j q_j^2$, to quantify the diversity of adversarial examples and a low value indicates less diversity. Here, $q_j \in (0, 1]$ is the probability of occurrence of the entity e_j among all instances of adversarial entities obtained from sampling, and $\sum_j q_j = 1$. A low diversity index indicates the reusability and is a proxy indicator for the universal adversarial attack regime (Moosavi-Dezfooli et al., 2017; Wallace et al., 2019a). Combining the ASR dependence on diversity and hyperparameter n in Fig. 2 reveals two regimes: (i) the adversarial entities semantically close to ($n < 0$) the key k have a greater diversity; (ii) the adversarial entities semantically far from ($n > 0$) the key k are more reusable. TCES in these two regimes both can lead to an increase in successful attacks from random sampling (equivalent to $n = 0$), as shown in Tables 1-2. Fig. 2 shows that a larger positive n in Eq. 2 samples more universal adversarial entities than in other situations, leading to a marked drop in the diversity index. Moreover, there exist local maxima of ASR in both regimes with finite

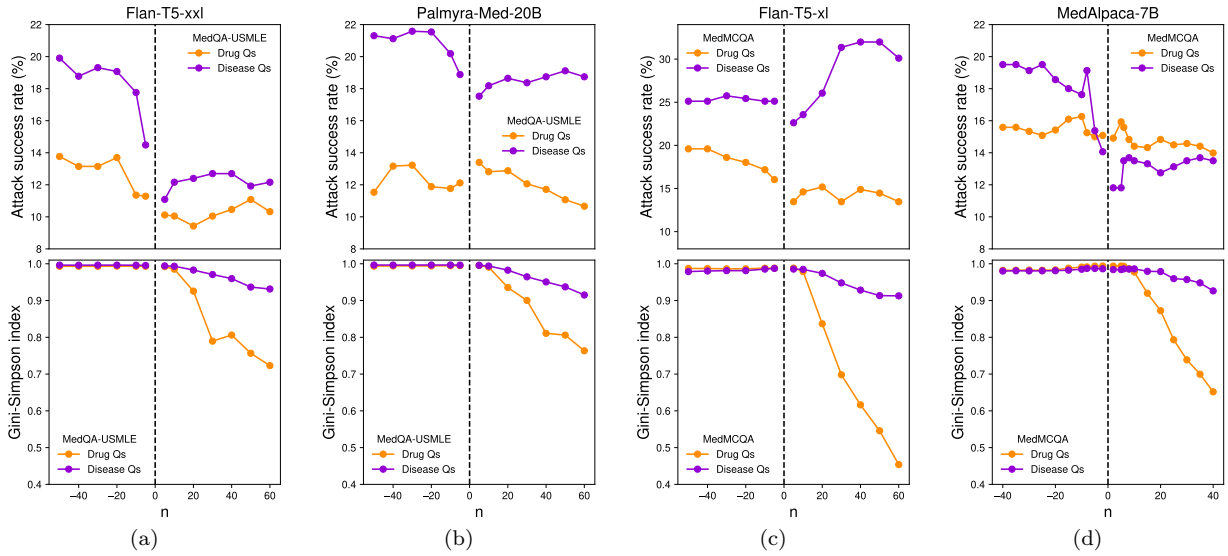


Figure 2: Powerscaled DWS of adversarial distractors exhibits a two-regime effect at negative and positive n values (see Eq. 2) in ASR (top) and diversity index (bottom) of replacement entities in successful attacks. Local maxima in ASR with a finite n are also present in each regime. The observed similar behaviors are compared across models and datasets in (a) Flan-T5-xxl on MedQA-USMLE, (b) Palmyra-Med-20B on MedQA-USMLE, (c) Flan-T5-xl on MedMCQA, (d) MedAlpaca-7B on MedMCQA. Disease and drug-mention questions are separated by colors. The vertical dashed line indicates the location of random sampling.

Model (size)	Entity mention	MedQA-USMLE			MedMCQA		
		Baseline (Acc)	RandS@1 (ASR %)	PDWS@1 (-/+) +CODER (ASR %)	Baseline (Acc)	RandS@1 (ASR %)	PDWS@1 (-/+) +CODER (ASR %)
Flan-T5-xl (3B)	Drugs	0.318	10.4	**13.5** / 10.7	0.265	14.3	**19.6** / 15.1
	Diseases	0.335	11.0	**16.1** / 12.5	0.261	23.8	25.7 / **31.8**
Flan-T5-xxl (11B)	Drugs	0.323	9.6	**13.6** / 11.2	0.291	12.7	**19.6** / 16.2
	Diseases	0.345	12.2	**20.0** / 12.8	0.376	15.2	**26.6** / 23.9
Flan-UL2 (20B)	Drugs	0.382	8.6	**12.3** / 10.5	0.416	13.9	**15.1** / 12.7
	Diseases	0.396	10.1	**15.7** / 13.1	0.408	15.7	**25.5** / 17.7
MedAlpaca-7B	Drugs	0.479	7.2	8.2 / **9.6**	0.448	13.9	**16.2** / 15.9
	Diseases	0.498	8.4	**12.5** / 9.2	0.434	14.8	**19.1** / 13.7
LM2-Medtuned-13B	Drugs	0.371	16.4	**18.1** / 17.8	0.568	15.3	17.3 / **18.1**
	Diseases	0.398	19.6	**23.1** / 19.6	0.515	19.0	**27.6** / 21.0
Palmyra-Med-20B	Drugs	0.382	12.6	13.3 / **13.5**	0.614	10.2	**13.8** / 12.7
	Diseases	0.441	16.9	**21.5** / 18.7	0.624	15.4	**20.1** / 11.9

Table 1: Single-query (budget = 1) attack success rates (ASRs) on subsets of MedQA-USMLE and MedMCQA datasets by perturbing the drug or disease entity mentions. Zero-shot baseline (Baseline) accuracy is included for reference next to the ASR of sampling attacks using perturbation by random sampling (RandS), powerscaled distance-weighted sampling (PDWS). The "-" and "+" signs indicate the two regimes ($n < 0$ and $n > 0$). For each model, the highest ASR for a type of entity-mention question in each dataset is bolded.

n, which were discovered by hyperparameter tuning. We call these behaviors the *two-regime effect* and they were observed in almost all models evaluated here in varying magnitudes for both QA datasets, thanks to the controllable spatial coverage of sampling methods incorporating distance information. In both single-query and multi-query attacks, the benchmarks show that the $n < 0$ regime of PDWS attacks tends to have a greater influence on model performance than the $n > 0$ regime, although prominent counterexamples do exist (MedAlpaca-7B and Llama2-Medtuned-13B (for drug-mention questions), and Flan-T5-xl (for disease-mention questions) in Table 1).

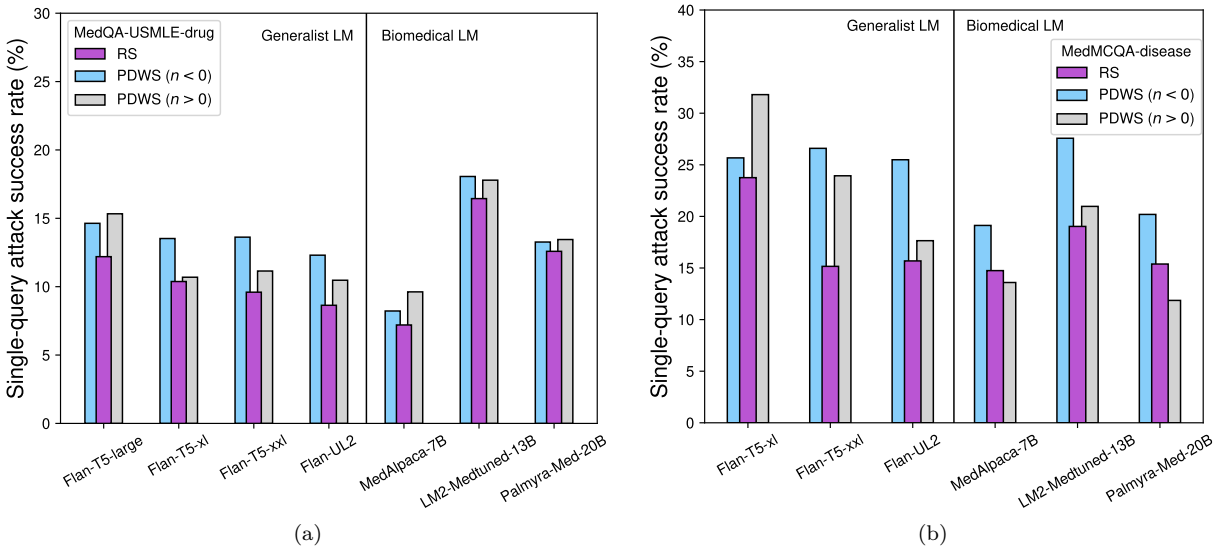


Figure 3: Model robustness from single-query adversarial attacks using results in Table 1. The models (GLMs and BLMs) were evaluated on drug-mention questions from MedQA-USMLE (left) and disease-mention questions from MedMCQA (right) datasets. The GLMs and BLMs are ordered horizontally by their sizes. The bar colors distinguish between different attack methods. Perturbations by random sampling (RS) are in purple. Perturbations by powerscaled DWS (PDWS) in the $n < 0$ and $n > 0$ regimes are in blue and grey, respectively.

Adversarial entity characteristics The two-regime effect indicates that the success of the attack may come from two sources. At small distances, semantic proximity (Mozes et al., 2021) reduces the distinguishability between the key and the distractor, therefore increasing the chance of model failure. Whereas at larger distances, the attack succeeds potentially due to the obscurity of the distractor entities in the question context, which can also profoundly impact the model performance (Li et al., 2023a). This explanation may be further supported by examining the diversity index, η_{GS}, which shows the dominance of a few replacement entities in successful attacks at large distances. We found these highly reusable adversarial entities by ranking their occurrences in successful attacks by powerscaled DWS. For drug names, the top-ranked adversarial entities include n-acetylglucosamine (an amino sugar and anti-inflammatory drug)[7] and technetium Tc 99m exametazime (a radiopharmaceutical and contrast agent)[8]. For disease names, some of the chromosome deletion syndromes and rare diseases names are more reusable than others. These entities dominate the sampling results in the $n > 0$ regime for all LLMs, indicating their transferability and universality.

5.2 Scaling characteristics from adversarial entities

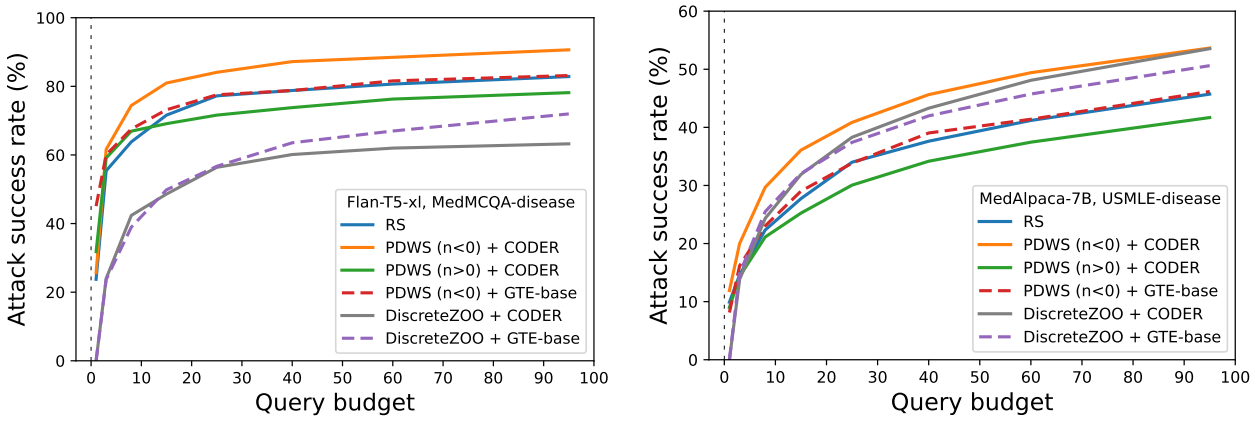
Size is not all for scaling model robustness. We compare model robustness using single-query ASR as the metric in Table 1 and Fig. 3. For the Flan-T5 series of GLMs (Chung et al., 2024) and Flan-UL2 (Tay et al., 2022), the single-query ASR is more pronounced in smaller and less performant models, indicating the improvement of robustness as the model's size grows. However, an opposite trend of robustness is seem in BLMs. It is worth noting that although Palmyra-Med-20B (Kamble & Alshikh, 2023) has about three times the number of parameters than MedAlpaca-7B (Han et al., 2023), the larger model is much more sensitive to entity perturbation. In terms of ASR, the BLMs are comparable to the GLMs in each type of questions evaluated on. Another observation is that the ASR for models is asymmetrical under PDWS attacks. For most of the models, sampling adversarial entities with inverse-distance-proportional weights ($n < 0$ in Eq. 2) induces more performance drop than sampling with distance-proportional weights ($n > 0$ in Eq. 2), yet prominent counterexamples exist. The attack performance is further investigated in the sequential, multi-

[7] n-acetylglucosamine on RxList
[8] technetium Tc 99m exametazime on RxList

query setting (budget = 8) in Table 2, where we also compared sampling- against search-based DiscreteZOO attacks. Here, PDWS attacks in the $n < 0$ regime are still largely the most effective.

Model (size)	Entity mention	MedQA-USMLE (ASR %)				MedMCQA (ASR %)			
		RandS @8	PDWS@8 (-/+) +CODER	DZOO@8 +CODER	DZOO@8 +GTE-base	RandS @8	PDWS@8 (-/+) +CODER	DZOO@8 +CODER	DZOO@8 +GTE-base
Flan-T5-xl (3B)	Drugs	22.0	**29.3** / 23.3	21.7	19.5	32.5	**48.3** / 36.2	34.3	28.2
	Diseases	27.2	**38.8** / 24.8	20.9	23.2	47.1	**61.7** / 49.0	45.8	39.3
Flan-UL2 (20B)	Drugs	22.5	**27.5** / 22.3	20.4	19.2	26.4	**35.6** / 22.4	30.7	26.4
	Diseases	25.8	**34.9** / 26.8	25.7	24.0	39.2	**49.5** / 31.6	41.3	37.0
MedAlpaca-7B	Drugs	16.8	21.1 / 22.3	**22.8**	20.5	27.9	37.1 / 30.1	**42.6**	36.8
	Diseases	21.7	**30.3** / 24.0	26.5	25.2	29.8	**43.9** / 30.8	40.5	38.1
Palmyra-Med-20B	Drugs	30.1	**31.4** / 31.3	29.1	29.6	28.5	**37.3** / 31.9	35.4	35.0
	Diseases	33.2	**35.1** / 30.2	32.3	34.5	41.1	48.4 / 39.6	46.3	**50.1**

Table 2: Multi-query (here budget = 8) attack success rates (ASR %) on various LLMs by perturbing the drug and disease entity mentions in MedQA-USMLE and MedMCQA datasets. The PDWS attack uses the embedding from CODER and DiscreteZOO (DZOO) attacks use either CODER or GTE-base embedding. For each model, the highest ASR for a type of entity-mention question in each dataset is bolded.



(a) (b)

Figure 4: Example scaling curves of the query budget against ASR for disease-mention questions with (a) Flan-T5-xl on MedMCQA dataset and (b) MedAlpaca model on MedQA-USMLE dataset. The curves are generated using TCES of disease names with the methods described in the legends. The DiscreteZOO attacks were run in the low-query-budget setting. Executing the random sampling (RS) attack doesn't require a text embedding, while the other attacks were evaluated with the CODER or GTE-base as text embedding.

Sampling attacks has improved query scaling over blackbox gradient attacks in specialized text embedding. A query scaling study of adversarial attacks investigates attack success with varying query budgets per input instance (Shukla et al., 2021). It is a comprehensive evaluation of attack methods. Fig. 4 compares the query scaling of both sampling- and search-based methods for TCES. For low-query-budget attacks (Fig. 1a), each scaling curve exhibits a rapid rise phase and a plateau phase, separated by an inflection point. The key message here is that the advantage of PDWS attacks over DiscreteZOO depends on the model and the choice of text embedding. The PDWS attacks are overarchingly more effective for GLMs than DiscreteZOO, while for BLMs, the advantage is reduced. Moreover, using a specialized text embedding further boosts the advantage of PDWS attacks compared with a general text embedding due to the difference in embedding space neighborhood. We expand the analysis in the following in three directions.

- **Query scaling depends on text embedding**: Changing the text embedding affects the query scaling behavior of both PDWS and DiscreteZOO attacks. Fig. 4 shows that the influence of the embedding choice on PDWS is more pronounced in the rapid rise phase, while it influences the DiscreteZOO primarily in the

A 73-year-old man presents to the outpatient clinic complaining of chest pain with exertion. He states that resting for a few minutes usually resolves the chest pain. Currently, he takes 81 mg of aspirin daily. He has a blood pressure of 127/85 mm Hg and heart rate of 75/min. Physical examination reveals regular heart sounds and clear lung sounds bilateral. Which medication regimen below should be added?

A: Amlodipine daily. Sublingual nitroglycerin as needed. B: Metoprolol and a statin daily. Sublingual nitroglycerin as needed. ✓ C: Metoprolol and ranolazine daily. Sublingual nitroglycerin as needed. D: Amlodipine and a statin daily. Sublingual nitroglycerin as needed.	A: Amlodipine daily. Sublingual nitroglycerin as needed. B: Metoprolol and a statin daily. Sublingual nitroglycerin as needed. C: N-acetylglucosamine and ranolazine daily. Sublingual nitroglycerin as needed. D: Amlodipine and a statin daily. Sublingual nitroglycerin as needed. ✓

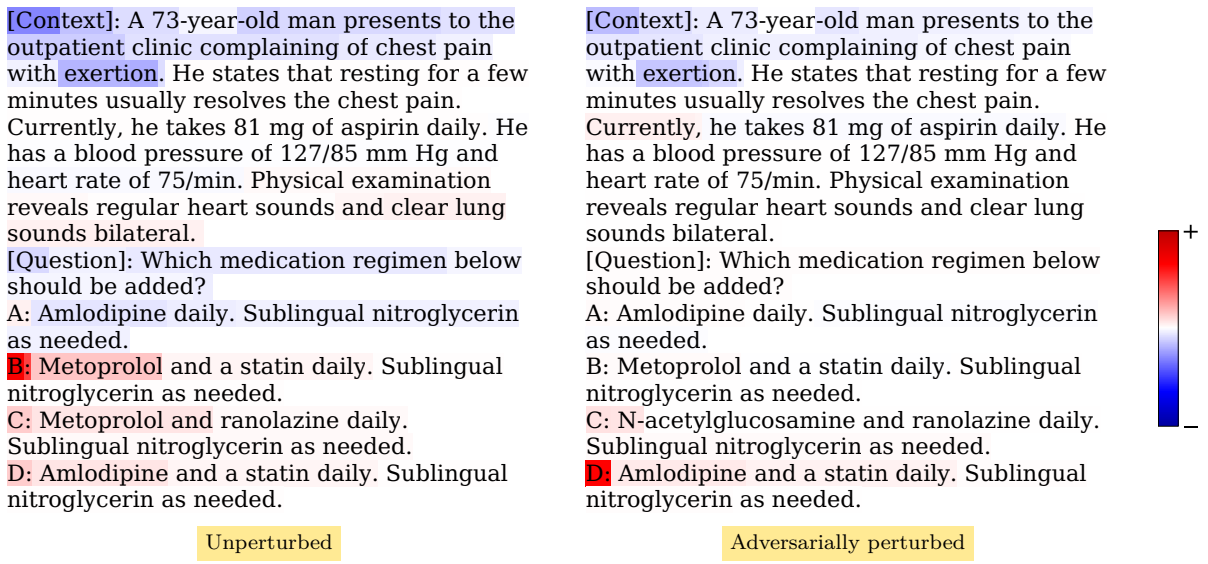


Figure 5: (Top) An entity substitution attack using n-acetylglucosamine as the replacement entity for metoprolol creates an adversarial distractor. (Bottom) Heatmaps of token-wise Shapley values for a question before and after the adversarial attack on option C. The model prediction changes from the correct choice of B (unperturbed) to the incorrect choice of D (adversarially perturbed).

plateau phase. Specifically, changing the text embedding from domain-specialized CODER (Yuan et al., 2022) to the general GTE-base (Li et al., 2023b), the performance advantage of PDWS over DiscreteZOO attacks shrunk in Flan-T5-xl (Fig. 4a) and inverted in MedAlpaca-7B (Fig. 4b).

- **Sampling hyperparameter controls scaling curve shape in PDWS attacks**: The hyperparameter n changes the inflection point of the scaling curve. When the query budget is past the inflection point of the curve, random sampling starts to surpass PDWS ($n > 0$) in ASR. This is a consequence of the distribution of adversarial entities in the embedding space and the regional bias derived from the sampling weights. The examples in Fig. 4 show that the largest performance gap between the PDWS and DiscreteZOO attacks appears at around the inflection point of the respective query scaling curve.
- **Gradient quality affects query scaling in DiscreteZOO attacks**: The query complexity in blackbox gradient estimation is a long-standing theoretical topic in derivative-free optimization (L'Ecuyer & Yin, 1998) and online learning (Duchi et al., 2015). Nevertheless, how gradient quality affects query scaling remains less studied for adversarial attacks employing gradient-based discrete optimization. Gradient estimation consumes a large part of the total query budget, leading to a tradeoff between the gradient quality and terminal ASR attainable (at max budget) in the query scaling curve. We empirically explored the query scaling behavior of the DiscreteZOO attack in Appendix E with different candidate points in

the multi-point gradient estimation, which in effect alters the gradient quality. The results show that having too few candidate points (i.e. small M in Eq. 5) leads to an early onset of the plateau phase, thereby limiting the highest attainable ASR, whereas having many candidate points can lead to a slower growth of ASR in the rapid rise phase of the query scaling curve.

5.3 Adversarial entities manipulate explainability

Post-hoc analysis is a common way to understand the rationale behind model decisions (Murdoch et al., 2019). Score-based feature importance such as that based on the Shapley values is routinely used to construct post-hoc explanation of model prediction through feature attribution (Chen et al., 2023). The stability of model explanation is a growing concern for their proper use (Alvarez-Melis & Jaakkola, 2018; Hancox-Li, 2020; Lin et al., 2023). Investigations on the susceptibility of LLM explanations to adversarial perturbation in QA are still lacking. For score-based feature importance, an explainer $\phi(\cdot)$ maps the m-dimensional feature $\mathbf{x} \in \mathbb{R}^m$ to scores $\phi(\mathbf{x}) \in \mathbb{R}^m$. In the current context, we assess the changes in feature importance represented by Shapley values (Chen et al., 2023) before ($\phi(\mathcal{Q})$) and after ($\phi(\mathcal{Q}')$) the adversarial attack by entity substitution $\mathcal{Q} \to \mathcal{Q}'$. For convenience of discussion, we use *Shapley profile* to refer to $\phi(\mathcal{Q})$ (or $\phi(\mathcal{Q}')$), the token-wise Shapley values calculated over $\mathcal{Q}$ (or $\mathcal{Q}'$).

We investigated the changes in the Shapley profile in the two regimes of adversarial entities for open-source LLMs, because the calculation requires access to model weights. We found that the token with the largest Shapley value (top-1 feature) is highly correlated with the model's prediction before and after adversarial perturbation, with an example shown in Fig. 5 produced using Flan-T5-large. This behavior is an indicator of the symbol-binding characteristic of LLMs in multiple-choice QA (Robinson & Wingate, 2023). Moreover, the Shapley profile typically exhibits pronounced changes before and after entity perturbation, especially in the text locations close to the perturbed entities (Fig. 5 and Appendix E). Together, these observations indicate that the substitution attacks effectively manipulate model explanations, because the explanation after the attack aligns with the wrong prediction, as if they were correct. The behavior occurs despite unchanged context, stem, and key ($\mathcal{C}$, $\mathcal{S}$, and k), which should contain the most important information for understanding and answering the question (Chai & Jin, 2004).

6 Discussion and future work

The present study illustrates that side information introduced through QA distractors can lead to noticeable performance degradation in billion-parameter LLMs. TCES with only a single entity modification step combined with adversarial sampling methods and appropriate text embeddings is a compact yet effective way for collecting adversarial entity data. Moreover, The perturbations from TCES appears natural to humans and are less likely to be detected using grammar check or topical filtering (Morris et al., 2020a). The setting simulates realistic scenarios where the "attacks" may be initiated by unsuspecting users, such as healthcare professionals using an LLM-based clinical decision support system (Liu et al., 2023). In the examples illustrated in Fig. 5 and Appendix E, adversarial distractors can lead to disease misdiagnosis or misprescription of medication, which are detrimental scenarios that may occur in algorithmic decision-making in biomedicine using LLMs. Further improvement on the sampling attack performance may be achieved using learned samplers through rejection mechanisms (Narasimhan et al., 2024) or by finetuning the text embedding to improve the query efficiency of sampling. Alternatively, the semantic distance used for sampling here may be replaced with a concept distance (Choi et al., 2016) to improve attack performance on general text embeddings. Our approach may be integrated into interactive platforms for adversarial data collection or testing in open-ended human-machine conversation (Chao et al., 2023) for online monitoring.

Future research may focus on how to make LLMs more reliable through prompt engineering (Si et al., 2023; Nori et al., 2023) or leveraging retrieval from nonparametric knowledge bases (Weikum et al., 2021; Soman et al., 2023) or text sources (Wang et al., 2023b) to improve model generalization to long-tail entities. Besides vulnerability identification, the current work motivates adversarial defense strategies based on generalized distances (La Malfa et al., 2020) to establish a tiered system for robustness assessment in user-facing and domain-oriented applications to mitigate catastrophic failures.

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