Zero-shot sampling of adversarial entities in biomedical question answering

Anonymous ACL submission

Abstract

The increasing depth of parametric domain knowledge in large language models (LLMs) is fueling their rapid deployment in real-world applications. In high-stakes and knowledge-intensive tasks, understanding model vulnerabilities is essential for quantifying the trustworthiness of model predictions and regulating their use. The recent discovery of named entities as adversarial examples in natural language processing tasks raises questions about their potential guises in other settings. Here, we propose a powerscaled distance-weighted sampling scheme in embedding space to discover diverse adversarial entities as distractors. We demonstrate its advantage over random sampling in adversarial question answering on biomedical topics. Our approach enables the exploration of different regions on the attack surface, which reveals two regimes of adversarial entities that markedly differ in their characteristics. Moreover, we show that the attacks successfully manipulate token-wise Shapley value explanations, which become deceptive in the adversarial setting. Our investigations illustrate the brittleness of domain knowledge in LLMs and reveal a shortcoming of standard evaluations for high-capacity models[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; Razniewski et al., 2021; 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 (Nat, 2023; Spitale et al., 2023; Si et al., 2023). Adversarial examples are valuable probes for model vulnerability and robustness, and are essential for performance evaluation and regulatory audits (Shayegani et al., 2023). 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 and Liang, 2017; Wallace et al., 2019b). While the search methods iteratively find random string adversarial examples (Wallace et al., 2019a), the sampling approach obviates the need for predetermined search heuristics. It can operate with only blackbox access to models and in the zero-shot setting, which is fitting for model auditing frameworks (Metaxa et al., 2021).

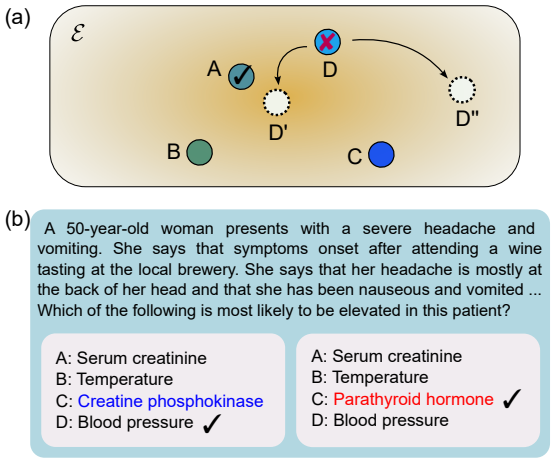


Figure 1: Text substitution attack on QA with adversarial distractors. (a) Illustration of the attack scheme in embedding space. A is the key to the question, B-D the original distractors, D′ and D″ the adversarial distractors semantically close to and far away from the key A, respectively. (b) An example of the attack showing the correct (left) and incorrect (right) model responses (checkmarked) before and after perturbation.

The present work focuses on question answering (QA) in the biomedical domain, which has been the proving ground in recent achievements of biomed-

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

ical language models (BLMs), here referring to GLMs adapted to the biomedical domain (Singhal et al., 2023a; Kung et al., 2023; Singhal et al., 2023b). GLMs have 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 from scholarly publications (Tinn et al., 2023). Although QA is frequently employed for model performance evaluation (Clark and Etzioni, 2016; Gardner et al., 2019; Robinson and Wingate, 2023), currently, the performance of LLMs in biomedical QA lacks systematic evaluation and their deployment in the real world is still in its infancy (Kung et al., 2023). Specifically, model performance against adversarial examples is seldomly assessed and their efficient sampling in the biomedical domain remains challenging, leaving a gap in our understanding of model robustness in entity-rich, high-stakes domain.

Knowledge and reasoning tests in the biomedical domain assess the understanding of diverse concepts, which are represented by domain-specific named entities (NEs). In this work, we develop an in-domain adversarial probe for model knowledge on biomedical NEs through text substitution of entity mentions in the distractors of multiple-choice QA. We introduce a powerscaled distance-weighted sampling (DWS) method in embedding space to generate adversarial examples of distractors, or *adversarial distractors*, in the zero-shot setting. Our work reports the first use of DWS for adversarial attacks in text[2]. The attack scheme enables traversing between the two regimes of adversarial entities semantically close to or far away from an anchor point (illustrated as the key A in Fig. 1a). For demonstration, we focus on attacking two of the most common NEs in the biomedical domain (Wei et al., 2019): drug and disease names, shown in an example in Fig. 1b.. In addition, we introduce 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). Through analysis of attack statistics, we show that our approach provides more flexibility to uniform random sampling in entity-centric attacks (Yan et al., 2022), which maps the entity-level robustness landscapes of different LLMs. We further explore the relationship between Shapley value-based model explanation (Chen et al., 2023) and adversarial attacks and uncover the defining signatures of successful attacks in this context.

[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).

2 Entity-centric adversarial attack

2.1 Adversarial distractor generation

We focus on constructing adversarial distractors in multiple-choice QA. Let 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 $\mathcal{S}$, 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 and 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

$$\mathcal{D}' = (\mathcal{D} \setminus \{d\}) \cup \{d'\}, \tag{1}$$

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 only contain NEs and each distractor involves only one NE (such as in Fig. 1b). An adversarially perturbed question elicits a false response from the model, while it answers correctly to the unperturbed question,

$$\begin{aligned} &\operatorname{argmax} \Pr(Y = k|\mathcal{C}, \mathcal{S}, \mathcal{D}', k) \\ &\qquad \neq \operatorname{argmax} \Pr(Y = k|\mathcal{C}, \mathcal{S}, \mathcal{D}, k). \end{aligned} \tag{2}$$

The formulation in Eq. (2) is an untargeted attack, while the targeted version only requires restricting the answer to the perturbed question to a specific distractor. We extend Eq. (2) to a more general case in Appendix A with multiple entities and additional text in the distractors. Unlike text addition attacks that introduce distracting information (Jia and Liang, 2017; Wallace et al., 2019a), the edit constraint on $\mathcal{Q}$ that is usually enforced in text adversarial attacks (Roth et al., 2021) 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 $\mathcal{E}_{\text{-}k} := \mathcal{E} \setminus \{k\}$, 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.

2.2 Powerscaled distance-weighted sampling

We consider sampling with distance-dependent probability weights from the embedding space of NEs. The concept of 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 in $\mathcal{E}_{\text{-}k}$ such that the distractor d is substituted by

$$d' = e_j \quad \text{w.p.} \quad p_j = \frac{h^n(k, e_j)}{\sum_j h^n(k, e_j)}. \qquad (3)$$

Here, $h(k, e_j)$ is a distance metric between 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, the entities closer to k are more preferably weighted. Besides, the formalism accommodates a deterministic regime as a limiting case[3]. It corresponds to $n \to +\infty$, when p_j is vanishingly small for all but the entity furthest from k in the embedding space according to $h(k, e_j)$,

$$d' = e_j \quad \text{s.t.} \quad e_j = \operatorname*{argmax}_{e_j \in \mathcal{E}_{\text{-}k}} h(k, e_j). \qquad (4)$$

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 Datasets

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 entities from known drugs approved by the United States Food and Drug Administration (FDA) and curated by Drug Central[4] (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[5] (`CTD-diseases`) contains over 9.8k 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. The 2023 version of the datasets was used after minor data processing.

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 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., 2023a; Han et al., 2023; Singhal et al., 2023b). 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 then divided the QA datasets into drug- or disease-mention questions by the binary mention labels generated according to the UMLS entity types. (see Appendix C).

4 Attack implementation

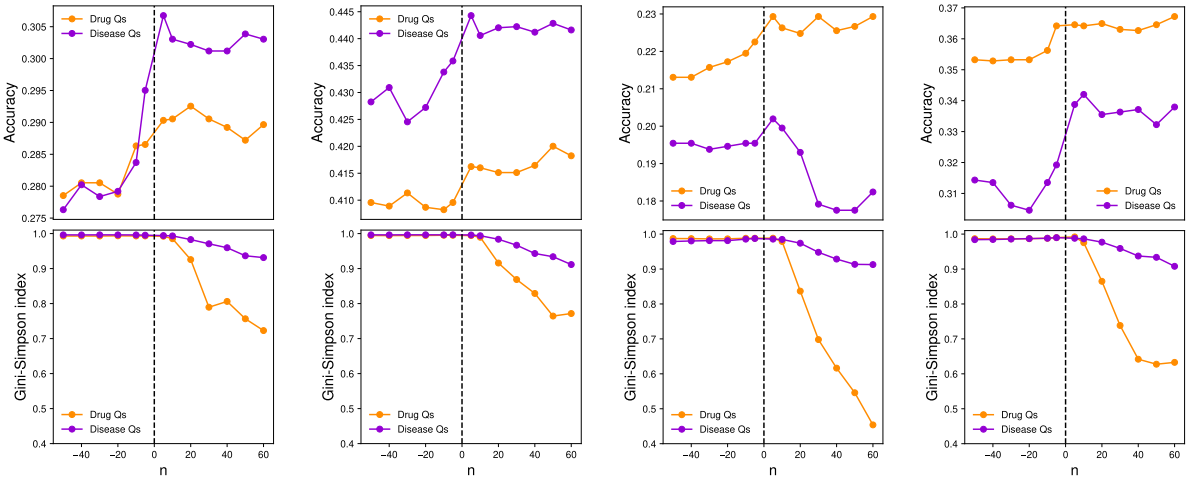
4.1 Type-constrained entity selection

Implementing the framework in Section 2 and Appendix A for drug and disease names requires accounting for the entity types they are associated with. We used the entity type annotations according to the UMLS (Bodenreider, 2004) of the semantic groups *Chemicals & Drugs* and *Disorders*. For each question the model answers correctly, we selected the entity of the same semantic group in

[3] 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.

[4] https://drugcentral.org/download

[5] https://ctdbase.org/downloads/



(a) (b) (c) (d)

Figure 2: Powerscaled DWS of adversarial distractors exhibits a two-regime effect at negative and positive n values (see Eq. (3)) in model accuracy (top) and diversity index (bottom) of replacement entities in successful attacks. The observed similar behaviors are compared across models and datasets in (a) Flan-T5-XXL on MedQA-USMLE, (b) MedAlpaca-7B on MedQA-USMLE, (c) Flan-T5-xl on MedMCQA, (d) Flan-UL2 on MedMCQA. Disease and drug-mention questions are separated by colors. The vertical dashed line indicates the location of random sampling.

the distractors closest to the key as the one to attack. The choice of the closest distractor is to maintain consistency and is not uniquely associated with the effects observed here. Then, we selected the replacement entity using random sampling or powerscaled DWS from the corresponding perturbation set $\mathcal{E}_{\text{-}k}$ (constructed with `FDA-drugs` or `CTD-diseases` datasets), which is equivalent to applying a type constraint to the replacement entity. For each question to attack, the probability weights in Eq. (3) were calculated for all members of $\mathcal{E}_{\text{-}k}$ using the cosine distance as h between the key and the replacement entities, k and e_j, in a surrogate word embedding of a BERT model finetuned on biomedical text (Yuan et al., 2022),

$$h(k, e_j) = 1 - \frac{\text{Embed}(k) \cdot \text{Embed}(e_j)}{\|\text{Embed}(k)\| \cdot \|\text{Embed}(e_j)\|}. \quad (5)$$

Using a shared embedding allows model evaluation by the same standard and simplifies the identification of transferable adversarial entities between models, as will be discussed in Section 5.

4.2 Attack execution on LLMs

We selected both generalist (GLMs) and specialist (BLMs) models for benchmarking sampling-based attacks, which require only API access to the LLM. For GLMs, we used instruction-finetuned T5 (Flan-T5) series of models (Chung et al., 2022) and UL2 model (Tay et al., 2022) (Flan-UL2), OpenAI's GPT-3.5 (text-davinci-003) (Brown et al., 2020) and Google's PaLM2 (text-bison-001) (Anil et al., 2023). For BLMs, we used MedAlpaca-7B (Han et al., 2023) and Writer's Palmyra-Med-20B (Kamble and Alshikh, 2023). The selected models contain diverse encoding schemes and architectures. Some of them have appeared on performance leaderboards of related tasks.

We assessed the performance of the LLMs at the baseline level and under sampling-based attacks, all in the zero-shot setting. This resulted in our somewhat lower baseline values than the reported model accuracies that are often achieved with the help of few-shot prompting and prompt optimization to improve performance. All models were evaluated at zero temperature or in the non-sampling setting. The prompts were structured as in Appendix D. Because only up to two model queries are required for each question, the computation is much more affordable than search-based approaches, which can take thousands or more queries (Alzantot et al., 2018). For the attack based on powerscaled DWS, we tuned the hyperparameter n within interval of [-50, 50] using a grid search. The interval was chosen for convenience because beyond this range, the performance drop that the attack incurred on the model doesn't deviate much from that at or within the interval boundaries.

5 Attack analysis and diagnostics

We conducted failure mode analysis using the attack statistics across models and the sampling hy-

Model (size)	Drug-mention questions			Disease-mention questions		
	NoPtb	RdPtb (↓%)	DistPtb- / DistPtb+ (↓%)	NoPtb	RdPtb (↓%)	DistPtb- / DistPtb+ (↓%)
Flan-T5-base (0.25B)	0.276	0.238 (13.8)	**0.230 (16.7)** / 0.235 (14.9)	0.260	0.226 (13.1)	**0.203 (21.9)** / 0.221 (15.0)
Flan-T5-large (0.78B)	0.287	0.252 (12.2)	0.245 (14.6) / **0.243 (15.3)**	0.294	0.249 (15.3)	0.230 (21.8) / **0.224 (23.8)**
Flan-T5-xl (3B)	0.318	0.285 (10.4)	**0.275 (13.5)** / 0.284 (10.7)	0.335	0.298 (11.0)	**0.281 (16.1)** / 0.293 (12.5)
Flan-T5-xxl (11B)	0.323	0.292 (9.6)	**0.279 (13.6)** / 0.287 (11.1)	0.345	0.303 (12.2)	**0.276 (20.0)** / 0.301 (12.8)
Flan-UL2 (20B)	0.382	0.349 (8.6)	**0.335 (12.3)** / 0.342 (10.5)	0.396	0.356 (10.1)	**0.334 (15.7)** / 0.344 (13.1)
GPT-3.5 (175B)	0.438	0.398 (9.1)	**0.389 (11.2)** / 0.391 (10.7)	0.453	0.414 (8.6)	**0.401 (11.5)** / 0.413 (8.8)
MedAlpaca-7B	0.460	0.431 (6.3)	0.421 (8.5) / **0.416 (9.6)**	0.488	0.439 (10.0)	**0.423 (13.3)** / 0.436 (10.7)
Palmyra-Med-20B	0.463	0.413 (10.8)	**0.405 (12.5)** / 0.414 (10.6)	0.500	0.441 (11.8)	**0.425 (15.0)** / 0.441 (11.8)
PaLM2 (350B)	0.287	0.263 (8.4)	**0.254 (11.5)** / 0.260 (9.4)	0.328	0.302 (7.9)	**0.283 (13.7)** / 0.297 (11.0)

Table 1: Adversarial testing of model performance on subsets of MedQA-USMLE dataset. Values outside parentheses are accuracies, those inside are percentage decreases (↓%) calculated using Eq. (6). NoPtb = unperturbed (baseline), RdPtb = perturbation by random sampling, DistPtb = perturbation by powerscaled DWS. The "-" and "+" signs indicate the two regimes ($n \ll 0$ and $n \gg 0$). The values for DistPtb- and DistPtb+ are found through hyperparameter tuning. For each model, the lowest accuracy for a type of questions is bolded.

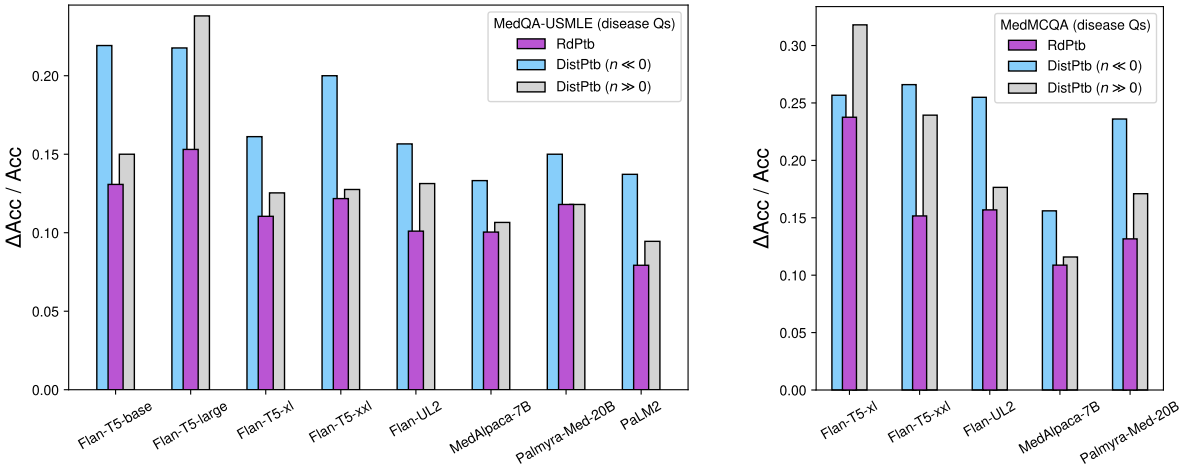
Model (size)	Drug-mention questions			Disease-mention questions		
	NoPtb	RdPtb (↓%)	DistPtb- / DistPtb+ (↓%)	NoPtb	RdPtb (↓%)	DistPtb- / DistPtb+ (↓%)
Flan-T5-xl (3B)	0.265	0.227 (14.3)	**0.213 (19.6)** / 0.225 (15.1)	0.261	0.199 (23.8)	0.194 (25.7) / **0.178 (31.8)**
Flan-T5-xxl (11B)	0.291	0.254 (12.7)	**0.234 (19.6)** / 0.244 (16.2)	0.376	0.319 (15.2)	**0.276 (26.6)** / 0.286 (23.9)
Flan-UL2 (20B)	0.416	0.358 (13.9)	**0.353 (15.1)** / 0.363 (12.7)	0.408	0.344 (15.7)	**0.304 (25.5)** / 0.336 (17.6)
MedAlpaca-7B	0.433	0.383 (11.5)	**0.381 (12.0)** / **0.381 (12.0)**	0.423	0.377 (10.9)	**0.357 (15.6)** / 0.374 (11.6)
Palmyra-Med-20B	0.675	0.602 (10.8)	**0.585 (13.3)** / 0.595 (11.9)	0.661	0.574 (13.2)	**0.505 (23.6)** / 0.548 (17.1)

Table 2: Adversarial testing of model performance on MedMCQA dataset (same structure as Table 1)

perparameter and through the effects on model explainability. The following summarizes the results.

Two regimes 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 $\sum_j q_j = 1$. The diversity index indicates the reusability of adversarial entities which we use as a proxy indicator for the universal adversarial attack regime (Moosavi-Dezfooli et al., 2017; Wallace et al., 2019a). By combining the accuracy and the diversity relations as n varies (Fig. 2), we uncover two regimes: (i) the adversarial entities semantically close to ($n \ll 0$) the key k have more diversity; (ii) the adversarial entities semantically far from ($n \gg 0$) the key k are more reusable. These two regimes both lead to an increase in successful attacks. Fig. 2 shows that a larger positive n in Eq. (3) samples more universal adversarial entities than in other situations, leading to a marked drop in the diversity index. We call this behavior the *two-regime effect* and it is observed in almost all models benchmarked on both QA datasets in varying magnitude.

The two-regime effect summarizes the observation that sampling with probability weights either proportional (positive n) or inversely proportional (negative n) to distance h produces adversarial entities more effectively than random sampling, as shown in Tables 1-2. The benchmarks show that the $n \ll 0$ regime tends to have a more detrimental influence on model performance than the $n \gg 0$ regime. Nevertheless, there exist prominent examples that go against the trend, such as MedAlpaca (for drug-mention questions) and Flan-T5-large in Table 1 and Flan-T5-xl (for disease-mention questions) in Table 2. At small distances, the success of the attack is related to semantic proximity (Mozes et al., 2021). Whereas at larger distances, the attack succeeds potentially due to the obscurity of the sampled entities in the question context, which may produce a profound impact on the model performance (Li et al., 2023). The reduction in the diversity index, η_{GS}, shows the dominance of a few replacement entities in successful attacks. We found the most reusable adversarial entities from



(a) (b)

Figure 3: Model robustness evaluated using R-CAP (ΔAcc/Acc) on disease-mention questions from (left) MedQA-USMLE and (right) MedMCQA datasets. The horizontal order partially reflects model performance without perturbation. The colors distinguishes entity-level perturbations by different sampling methods. Perturbations by random sampling (RdPtb) are in purple. Perturbations by powerscaled DWS (DistPtb) in the $n \ll 0$ and $n \gg 0$ regimes are in blue and grey, respectively. A lower value of ΔAcc/Acc indicates a more robust model.

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)[6] and technetium Tc 99m exametazime (a radiopharmaceutical and contrast agent)[7]. 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 $n \gg 0$ regime for all LLMs, indicating their transferability and universality. An example attack using n-acetylglucosamine as recommended medication is in Fig. 4. Adversarial entities in the $n \ll 0$ regime have improper spellings such as missing possessives or they are insufficiently detailed.

Size is not all for model robustness. A typical metric for model robustness assessment is the change in accuracy before and after perturbation (Zhang et al., 2022). To enable comparison between datasets, we quantify the model robustness through its relative change in accuracy (Acc) upon perturbation (R-CAP), as shown partly in Fig. 3.

$$\frac{\Delta\text{Acc}}{\text{Acc}} = \frac{\Delta(n_{\text{TP}} + n_{\text{TN}})}{n_{\text{TP}} + n_{\text{TN}}} \quad (6)$$

R-CAP is equivalently the relative change in the number of correct model predictions (numbers of true positives n_{TP} and true negatives n_{TN}) (Wang et al., 2023b). Tables 1-2 show that zero-shot adversarial sampling already incurs about 10-20% of relative change in accuracy. For the Flan-T5 series (Chung et al., 2022), R-CAP is more pronounced for smaller and less performant models, indicating the improvement of robustness as models scale up. However, the BLMs are generally more robust to entity substitution than GLMs for models of a similar size. The trend is consistent in both of the two regimes found through hyperparameter tuning of the powerscaled DWS. It is worth noting that although Palmyra-Med-20B (Kamble and Alshikh, 2023) has about three times the number of parameters than MedAlpaca-7B (Han et al., 2023), it is much more sensitive to entity perturbation. Therefore, the smaller BLM is more robust against perturbation. Another observation is that the R-CAP for models upon adversarial perturbations is asymmetrical. For most of the models, sampling adversarial entities closer to the key induces more performance drop than sampling further away.

Entity substitution attacks 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 are 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 and Jaakkola, 2018; Hancox-Li, 2020; Lin

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

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. ✓

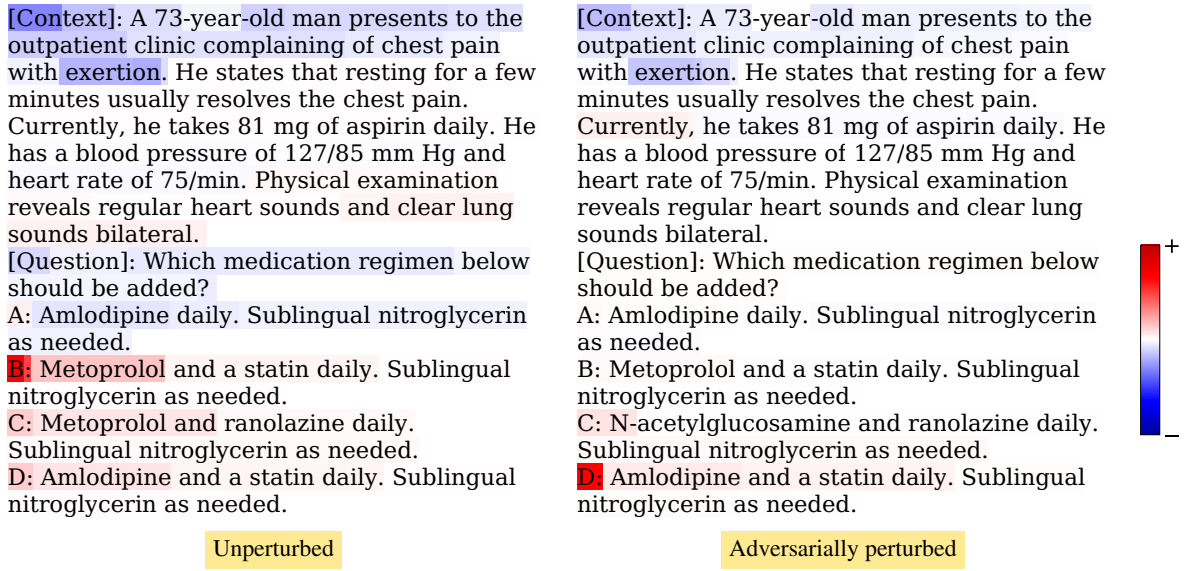


Figure 4: (Top) An entity subsitution attack using n-acetylglucosamine as the replacement entity for metoprolol creates an adversarial distractor. (Bottom) Heatmaps of token-wise Shapley values for a question before and after the adversarial attack on option C. The model prediction changes from the correct choice of B (unperturbed) to the incorrect choice of D (adversarially perturbed).

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 $\mathcal{Q} \rightarrow \mathcal{Q}'$. 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. 4 produced using Flan-T5-large. This behavior is an indicator of the symbol-binding characteristic of LLMs in multiple-choice QA (Robinson and 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. 4 and Appendix E). Together, these observations indicate that the substitution attacks effectively manipulate model explanations, because the explanation after 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 and Jin, 2004).

6 Related works

Text substitution attack 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). Alzantot et al. (2018) used a genetic algorithm to search for adversarial word substitution. Model sensitivity to entity-level perturbations such as substitution and swapping create problematic situations for knowledge-intensive tasks, such as knowledge conflicts (Longpre et al., 2021), 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 systems has been studied using perturbative methods (Jia and Liang, 2017) and meaning-preserving transformations (Gan and Ng, 2019; Elazar et al., 2021). Sen and Saffari (2020) introduced a set of perturbations to assess language model generalization between QA datasets. Richardson and 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 and Hruschka, 2023; Zheng et al., 2023). Overall, the brittleness of knowledge in LLMs remains a primary limitation for their applications (Razniewski et al., 2021; Elazar et al., 2021; Ji et al., 2023).

Adversarial attack characteristics The defining characteristic of adversarial attacks is to induce false predictions in trained models. Besides, attacks may possess transferability, universality (Zou et al., 2023), and they may obstruct model explanation (Noppel and Wressnegger, 2024). Transferability refers to the effectiveness of the same example being adversarial to a number of 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). Model explanations may be manipulated by specifically designed perturbations to the inputs (Dombrowski et al., 2019) or biased data subsampling (Laberge et al., 2023).

7 Discussion and future work

The present study illustrates that side information introduced through entity substitution leads to noticeable degradation of model performance, by modifying only a single sampling step and without gradient computation. Moreover, type-constrained entity substitution makes sure that the replacement entity appears natural to human and is less likely to be detected using grammar check or topical filtering (Morris et al., 2020). The setting simulates realistic scenarios where the “attacks" may be initiated by unsuspecting users, such as biomedical professionals using an LLM-based clinical decision support system (Liu et al., 2023). In the examples illustrated in Fig. 4 and Appendix E, adversarial distractors can lead to disease misdiagnosis or prescription of the wrong medication, which are detrimental scenarios that may occur in algorithmic decision-making in biomedicine. Further improvement on the attack performance may be achieved by sequential sampling, an intrinsic approach to boost the sampling performance, or by changing the entity vocabulary of the perturbation set, an extrinsic approach that depends on the user and application setting. Our approach may be integrated into interactive platforms for adversarial testing in open-ended human-machine conversation (Chao et al., 2023) for online model auditing.

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., 2023c) to improve model generalization to long-tail entities. The DWS methodology may be extended to kernel methods (Hofmann et al., 2008) or metric learning (Bellet et al., 2015), which can capture more general distance dependence. Besides vulnerability identification, the current work motivates adversarial defense strategies based on generalized distances to establish a tiered system for validating adversarial robustness in user-facing and domain-oriented applications.

Limitations

Although NEs convey parts of the key information in the question, they fall short of capturing the entirety of the textual meaning. To explore other attack surfaces within the adversarial landscape of QA, one would need to evaluate the robustness in multidimensional perturbation space (Wang et al., 2022). Besides, the meaning of Shapley values calculated here requires additional interpretation due to feature correlation. Although we use them in part to reveal the importance of specific tokens, their robustness is also worth exploring using sentence-level features (Chen et al., 2023).

Ethics statement

The scenarios considered in this work using public datasets relate to potential real-world deployment of LLMs in biomedical education and clinical decision support. Our results show that the lack of adversarial testing methods in high-stakes domains may incur serious consequences because of naturally looking adversarial examples. The design and deployment of adversarial testing should be specific to and carried out at every stage of the model development cycle, paired with tools such as adversarially robust model explainability methods for understanding model behavior.

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A Adversarial distractor generation

We formulate here the general case of adversarial distractor generation when the choices contain text other than entities and one or more entities are present in a single choice. To keep the symbols consistent with Section 2, we let the question be $\mathcal{Q} = (\mathcal{C}, \mathcal{S}, \mathcal{D}, \mathcal{K})$, with the context $\mathcal{C}$, question stem $\mathcal{S}$. We write the distractor set $\mathcal{D} = \{\mathcal{D}_i\}_{i=1}^{l}$, and each distractor $\mathcal{D}_i$ contains a set of entities $\{d_{i,j}\}_{j=1}^{l_i}$ and additional text, which means that

$$\mathcal{D}_i \setminus (\cup_j \{d_{i,j}\}) \neq \varnothing. \tag{7}$$

The key $\mathcal{K}$ contains the entity k and other text. We use the notation $\mathcal{Q}(d_{i,j} \rightarrow d'_{i,j})$ to denote that a distractor entity $d_{i,j}$ is substituted by $d'_{i,j}$ in the questions $\mathcal{Q}$. If $d_{i,j}$ in the question is adversarially perturbed, the model elicits a false response, while it answers correctly to the unperturbed question $\mathcal{Q}$,

$$\begin{aligned} &\operatorname{argmax} \Pr(Y = \mathcal{K} | \mathcal{Q}(d_{i,j} \rightarrow d'_{i,j})) \\ &\qquad \neq \operatorname{argmax} \Pr(Y = \mathcal{K} | \mathcal{Q}). \end{aligned} \tag{8}$$

The general case is reduced to the special case described in Section 2 when $l_i = 1$, $\mathcal{D}_i = d_{i,1} := d_i$, and $\mathcal{K} = k$, which recover $\mathcal{D} = \{d_i\}_{i=1}^{l}$, and $\mathcal{Q} = (\mathcal{C}, \mathcal{S}, \mathcal{D}, k)$.

B Proof of the sampling regimes

Here we present a simple proof of the deterministic limit of the powerscaled distance-weighted sampling described in Eq. (3) of the main text. Although the distance function h is not given a specific form, we assume it to satisfy the basic properties of a metric. Given a perturbation set $\mathcal{E}_{\text{-}k} = \{e_1, ..., e_m\}$ with respect to a key k, there exists a corresponding set of distance values $\mathcal{H}_{\text{-}k}$.

B.1 The limit of $n \rightarrow +\infty$

We order the elements of $\mathcal{H}_{\text{-}k}$ and define the ordered set $\mathcal{H}_{\text{-}k,\uparrow} = \{h_{1,\uparrow}, ..., h_{m,\uparrow}\}$ such that,

$$h_{i,\uparrow} < h_{j,\uparrow} \quad \text{iff} \quad i < j \tag{9}$$

This indicates that $h_{m,\uparrow} = \max \mathcal{H}_{\text{-}k,\uparrow}$, and $h_{j,\uparrow}/h_{m,\uparrow} < 1$ for any $j \neq m$. We compute the probability weights as $n \rightarrow +\infty$ for each entity $e_j \in \mathcal{E}_{\text{-}k}$. When $j \neq m$,

$$\begin{aligned} \lim_{n\rightarrow+\infty} p_{j,\uparrow} &= \lim_{n\rightarrow+\infty} \frac{h_{j,\uparrow}^n}{\sum_j h_{j,\uparrow}^n} \\ &= \lim_{n\rightarrow+\infty} \frac{(h_{j,\uparrow}/h_{m,\uparrow})^n}{\sum_{j\neq m}(h_{j,\uparrow}/h_{m,\uparrow})^n + (h_{m,\uparrow}/h_{m,\uparrow})^n} \\ &= \frac{0}{0+1} = 0. \end{aligned} \tag{10}$$

Similarly, as $n \rightarrow +\infty$, the probability weight for the mth entity is

$$\lim_{n\rightarrow+\infty} p_{m,\uparrow} = 1. \tag{11}$$

For the entities in the perturbation set $\mathcal{E}_{\text{-}k}$, this indicates that only

$$e_j = \operatorname{argmax} \mathcal{H}_{\text{-}k,\uparrow} = \operatorname*{argmax}_{e_j \in \mathcal{E}_{\text{-}k}} h(k, e_j) \tag{12}$$

is selected with certainty at the deterministic limit.

B.2 The limit of $n \rightarrow -\infty$

A similar approach to B.1 can be used to construct the probability weights in the limit $n \rightarrow -\infty$. As noted in the footnote of the main text, this limit is not attained since $k \notin \mathcal{E}_{\text{-}k}$.

B.3 The case of $n = 0$

When $n = 0$, it is straightforward to show that $p_j|_{n=0} = 1/m$, regardless of j using the definition in Eq. (3). This scenario therefore corresponds to uniform random sampling.

C Biomedical entity processing

The original `MedQA-USMLE` (Jin et al., 2021) and `MedMCQA` (Pal et al., 2022) datasets lack entity annotations. In the present work, we carried out a two-step annotation for both datasets.

UMLS entity types We annotated the datasets using the type unique identifiers (TUIs) specified in the UMLS (Bodenreider, 2004) for biomedical entities. The annotation produces TUIs and the entity boundaries for entire questions and was carried out using `scispaCy` (Neumann et al., 2019) with the `en_core_sci_md` model. The annotation should be regarded as algorithmically produced, rather than human-annotated and proofread ground truth.

Prompt format

Answer the following question without explanation.

[Content]: A 23-year-old pregnant woman at 22 weeks gestation presents with burning upon urination. She states it started 1 day ago and has been worsening despite drinking more water and taking cranberry extract. She otherwise feels well and is followed by a doctor for her pregnancy. Her temperature is 97.7°F (36.5°C), blood pressure is 122/77 mmHg, pulse is 80/min, respirations are 19/min, and oxygen saturation is 98% on room air. Physical exam is notable for an absence of costovertebral angle tenderness and a gravid uterus.

[Question]: Which of the following are the best treatment for this patient?
A: Ampicillin
B: Ceftriaxone
C: Doxycycline
D: Nitrofurantoin

[Answer]:

Binary mention labels For entity-level perturbation, the distinction between questions with and disease entity mentions is based on the type of entities present in the distractors. We generate the binary mention labels ("Drugs?" and "Diseases?") for each question selected from the two datasets using the UMLS semantic groups of the TUIs in (i) for the distractors. Specifically, a drug-mention question has one or more entities in the distractors of the *Chemicals & Drugs* semantic group. A disease-mention question has one or more entities of the *Disorders* semantic group in its distractors.

D Prompt formatting

We structured the prompt with bracketed tags to divide different parts (Context, Question, Answer). An example taken from the MedQA-USMLE dataset (Jin et al., 2021) is shown below. For the MedMCQA dataset (Pal et al., 2022), only the Context and Answer[1] tags were used because the questions are short and generally contain no context. The prompt formatting improves model performance and facilitates answer parsing in the model-generated text. The increased space between paragraphs in the following is only to assist viewing and is not included in the actual prompt.

E Model evaluation and attack examples

We list some examples of successful entity substitution attacks using adversarial distractors following Fig. 4 in the main text. For each example, the text box on top (the prompt formatting removed) shows the original options on the left side and the perturbed options on the right side. The entity of interest before and after perturbation is colored in red and blue, respectively. The checkmark indicates the model prediction on unperturbed and perturbed questions. Beneath the text box are the corresponding heatmaps of token-wise Shapley values (or Shapley profile) before and after the entity substitution attack. The Shapley profiles for the MedQA-USMLE dataset (Jin et al., 2021) were generated using the model Flan-T5-large and those for the MedMCQA (Pal et al., 2022) using the model Flan-T5-xxl (Chung et al., 2022). The Shapley values were calculated using the partition explainer in `shap`, which uses the Owen values as an approximation (Chen et al., 2023).

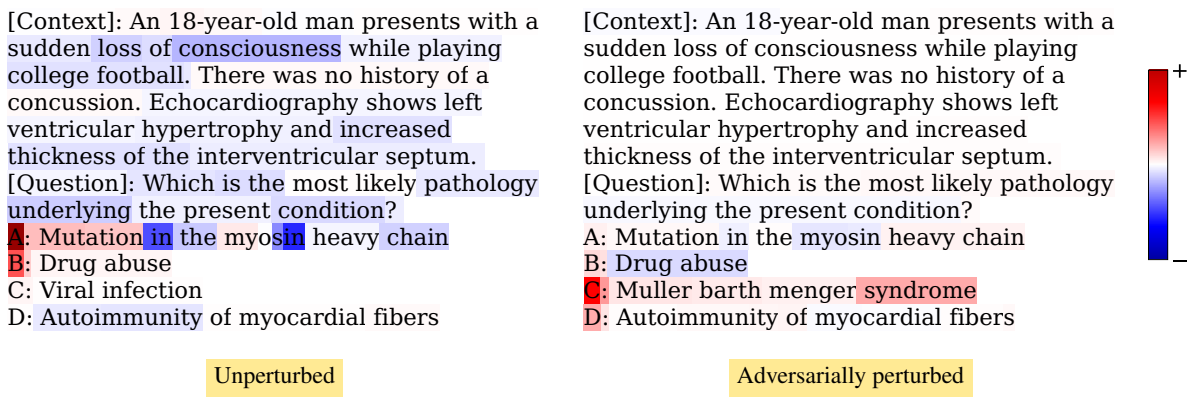
Of the LLMs evaluated in this work, the proprietary models (GPT-3.5, PaLM2) were accessed through third-party APIs, while the open-source models were accessed on local cache to improve speed. The evaluations were carried out on a variety of NVIDIA GPUs depending on the model size. For smaller model such as the Flan-T5 series (Chung et al., 2022), the runtime on each type of questions (involving drug or disease mentions) in a dataset was generally between 10 and 30 minutes, while it was from one to more than four hours for larger model such Flan-UL2 (Tay et al., 2022) and Palmyra-Med-20B (Kamble and Alshikh, 2023). For proprietary models accessed through their APIs, the runtime for each type of questions is between two and four hours.

[1] Using the Context tag improves model performance than the Question tag here.

MedQA-USMLE

An 18-year-old man presents with a sudden loss of consciousness while playing college football. There was no history of a concussion. Echocardiography shows left ventricular hypertrophy and increased thickness of the interventricular septum. Which is the most likely pathology underlying the present condition?

A: Mutation in the myosin heavy chain ✓	A: Mutation in the myosin heavy chain
B: Drug abuse	B: Drug abuse
C: Viral infection	C: Muller barth menger syndrome ✓
D: Autoimmunity of myocardial fibers	D: Autoimmunity of myocardial fibers



MedQA-USMLE

A 41-year-old woman comes to the physician because of a 3-month history of anxiety, difficulty falling asleep, heat intolerance, and a 6-kg (13.2-lb) weight loss. The patient's nephew, who is studying medicine, mentioned that her symptoms might be caused by a condition that is due to somatic activating mutations of the genes for the TSH receptor. Examination shows warm, moist skin and a 2-cm, nontender, subcutaneous mass on the anterior neck. Which of the following additional findings should most raise concern for a different underlying etiology of her symptoms?

A: Nonpitting edema ✓	A: Nonpitting edema
B: Atrial fibrillation	B: Atrial fibrillation
C: Lid lag	C: Lid lag
D: Fine tremor	D: Nonpuerperal galactorrhea ✓

[Context]: A 41-year-old woman comes to the physician because of a 3-month history of anxiety, difficulty falling asleep, heat intolerance, and a 6-kg (13.2-lb) weight loss. The patient's nephew, who is studying medicine, mentioned that her symptoms might be caused by a condition that is due to somatic activating mutations of the genes for the TSH receptor. Examination shows warm, moist skin and a 2-cm, nontender, subcutaneous mass on the anterior neck.
[Question]: Which of the following additional findings should most raise concern for a different underlying etiology of her symptoms?
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Adversarially perturbed

MedQA-USMLE

A 25-year-old man is brought to the emergency department after his girlfriend discovered him at home in a minimally responsive state. He has a history of drinking alcohol excessively and using illicit drugs. On arrival, he does not respond to commands but withdraws all extremities to pain. His pulse is 90/min, respirations are 8/min, and blood pressure is 130/90 mm Hg. Pulse oximetry while receiving bag-valve-mask ventilation shows an oxygen saturation of 95%. Examination shows cool, dry skin, with scattered track marks on his arms and legs. The pupils are pinpoint and react sluggishly to light. His serum blood glucose level is 80 mg/dL. The most appropriate next step in management is intravenous administration of which of the following?

A: Naloxone
B: Phentolamine ✓
C: Methadone
D: Naltrexone

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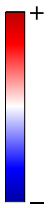

MedQA-USMLE

A 70-year-old woman presents to the office for a yearly physical. She states she has recently started experiencing pain in her legs and her back. Last year, she experienced a fracture of her left arm while trying to lift groceries. The patient states that she does not consume any dairy and does not go outside often because of the pain in her legs and back. Of note, she takes carbamazepine for seizures. On exam, her vitals are within normal limits. You suspect the patient might have osteomalacia. Testing for which of the following is the next best step to confirm your suspicion?

A: 25-hydroxyvitamin D ✓
B: 1,25-hydroxyvitamin D
C: Pre-vitamin D3
D: Dietary vitamin D2

A: 25-hydroxyvitamin D
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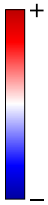

MedMCQA

Which of the following is granted orphan drug status for the treatment of Dravet's syndrome?

A: Stiripentol
B: Icatibant
C: Pre-vitamin D3
D: Tafamidis ✓

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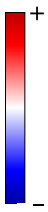

MedMCQA

Which among the following may be used as a sedatives-hypnotic?

A: Zolmitriptan
B: Zileuton
C: Zolpidem ✓
D: Zalcitabine

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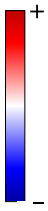
Adversarially perturbed