# Counterfactual Token Generation in Large Language Models

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#### Abstract

"Sure, I am happy to generate a story for you: Captain Lyra stood at the helm of her trusty ship, the Maelstrom's Fury, gazing out at the endless sea. [...] Lyra's eyes welled up with tears as she realized the bitter truth – she had sacrificed everything for fleeting riches, and lost the love of her crew, her family, and herself." Although this story, generated by a large language model, is captivating, one may wonder-how would the story have unfolded if the model had chosen "Captain Maeve" as the protagonist instead? We cannot know. State-of-the-art large language models are stateless—they maintain no internal memory or state. Given a prompt, they generate a sequence of tokens as an output using an autoregressive process. As a consequence, they cannot reason about counterfactual alternatives to tokens they have generated in the past. In this work, our goal is to enhance them with this functionality. To this end, we develop a causal model of token generation that builds upon the Gumbel-Max structural causal model. Our model allows any large language model to perform counterfactual token generation at almost no cost in comparison with vanilla token generation, it is embarrassingly simple to implement, and it does not require any fine-tuning nor prompt engineering. We implement our model on Llama 3 8B-instruct and conduct both qualitative and quantitative analyses of counterfactually generated text. We conclude with a demonstrative application of counterfactual token generation for bias detection, unveiling interesting insights about the model of the world constructed by large language models.

## 1 Introduction

Reasoning about "what might have been", about alternatives to our own past actions, is a landmark of human intelligence [1-3]. This type of reasoning, known as counterfactual reasoning, has been shown to play a significant role in the ability that humans have to learn from limited past experience and improve their decision making skills over time [4-6], it provides the basis for creativity and insight [7], and it is tightly connected to the way we attribute causality and responsibility [8–11]. Can currently available large language models (LLMs) conduct counterfactual reasoning about alternatives to their own outputs? In this work, we argue that they cannot, by design.

Currently available LLMs are stateless—they maintain no internal memory or state. Given an input prompt, they generate a sequence of tokens<sup>1</sup> as output using an autoregressive process [12, 13]. At each time step, they first use a neural network to map the prompt and the (partial) sequence of tokens generated so far to a token distribution. Then, they use a sampler to draw the next token at random from the token distribution.<sup>2</sup> Finally, they append the next token to the (partial) sequence of tokens, and continue until

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 $<sup>^{1}</sup>$ Tokens are the units that make up sentences and paragraphs. Examples of tokens include (sub-)words, symbols, numbers, and special end-of-sequence tokens.

<sup>&</sup>lt;sup>2</sup>Multiple lines of evidence suggest that, if a LLM is forced to output tokens deterministically, its performance worsens [14].



Figure 1: Illustrative examples of autoregressive token generation. In all panels, plain text indicates the input provided to the LLM and highlighted text indicates the output generated by the model. Each token in the output sequence is highlighted in a different color to represent the (stochastic) state of the sampler. Panel (a) shows an LLM's output to a user's prompt using vanilla autoregressive token generation. Panels (b, c) show an LLM's output to an input comprising a user's prompt and an unmodified/modified part of the original output from Panel (a) using vanilla autoregressive token generation. Panel (d) shows an LLM's counterfactual output to an input comprising a user's prompt and a modified part of the output from Panel (a) using autoregressive token generation. Panel (a) using autoregressive token generation augmented with the Gumbel-Max SCM.

a special end-of-sequence token is sampled. To understand why this autoregressive process is insufficient to reason counterfactually about alternatives to a previously generated sequence of tokens, we will use an illustrative example.

Consider that we ask an LLM to share its favorite color, as shown in Figure 1a. Had the LLM chosen a different color (*e.g.*, purple instead of blue), what would the rest of its output have been? To answer such a counterfactual question, we need to implement two actions: (i) modify the (partial) sequence of tokens fed to the neural network used by the LLM and (ii) compel the sampler used by the LLM to behave exactly as it did in the original generation. Using currently available LLMs, we can readily implement the first action, which can be viewed as a causal intervention [15, 16]. We just need to replace "blue" with "purple" in the (partial) sequence of tokens fed to the neural network. However, we cannot easily implement the second action, because the sampler does not specify how it would have behaved after taking the first action while keeping everything else equal. In fact, note that, if we provide the (modified) partial sequence up to and including the world "blue" ("purple") as input to the LLM, there is no way to ensure that the LLM will generate an output that matches (the structure of) the original output because the (stochastic) state of the sampler is different, as shown in Figures 1b and  $1c.^3$ 

**Our contributions.** Our key idea is to augment the autoregressive process underpinning an LLM, particularly the sampler used in the process, using the Gumbel-Max structural causal model (SCM) [17]. Under this model, the sampler is defined through a causal mechanism which receives as an input the distribution of the next token and a set of Gumbel noise values. Importantly, this causal mechanism specifies how the sampler would have behaved under an intervention on the distribution of the next token and thus allows us to answer counterfactual questions about a previously generated sequence of tokens, as shown in Figure 1d. Along the way, we also introduce an efficient implementation of the augmented autoregressive process that can generate counterfactual tokens at almost no cost in comparison with vanilla token generation. As a proof of concept, we implement our model on Llama 3 8B-instruct, and we conduct experiments to qualitatively and quantitatively analyze the similarity between an LLM's original output and the one generated via counterfactual token generation. Additionally, we demonstrate the use of our methodology for bias detection, unveiling interesting insights about the model of the world constructed by large language models. An open-source implementation of our model on Llama 3 8B-instruct is available at https://github.com/Networks-Learning/counterfactual-11ms.

 $<sup>^{3}</sup>$ Note that using the same random seed is not sufficient because the inputs in Figure 1a and Figures 1b and 1c differ in their number of tokens.

**Further related work.** Our work is most closely related to a line of work on counterfactual text generation [18–27]. In this line of work, given pairs of factual statements and interventions over these statements, the goal is to generate counterfactual statements that match those made by humans—counterfactual statements that are consistent with the underlying model of the world shared by humans. To this end, existing methods typically fine-tune an LLM using a dataset comprising factual statements, interventions over these statements, and counterfactual statements made by humans. In contrast, in our work, our goal is to generate counterfactual statements that are consistent with the underlying model of the world constructed by a given LLM [28–31]. In this context, our work also relates to a rapidly increasing number of empirical studies assessing the ability of LLMs to answer questions that require counterfactual reasoning [32–43]. Here, the LLMs are typically evaluated using multiple choice questions about a given set of factual and counterfactual statements. However, similarly as in the line of work on counterfactual text generation discussed previously, the counterfactual statements are made by humans.

The Gumbel-max structural causal model has previously been used to enable counterfactual reasoning in Markov decision processes [44], temporal point processes [45], and expert predictions [46]. However, to the best of our knowledge, it has not been previously used to enable counterfactual reasoning in LLMs.

### 2 A Causal Model of Token Generation

To formally express autoregressive token generation, we adopt (part of) the notation introduced by Duetting et al. [47] in a different (non-causal) context. Let V denote the vocabulary (set) of tokens available to the LLM, which includes an end-of-sequence token  $\bot$ . Then, we denote by  $V^* = V \cup V^2 \cup \cdots \cup V^K$  the set of sequences of tokens up to maximum length K, and by  $\emptyset$  the empty token. An LLM takes as input a prompt sequence  $s_q \in V^*$  and responds with an output sequence  $s \in V^*$ . The output sequence is generated using an autoregressive process. At each time step  $i \in [K]$ , the LLM first takes as input the concatenation of the prompt sequence  $s_q$  and the (partial) output sequence  $s_{i-1}$  and generates a distribution over tokens  $d_i \in \Delta(V)$ . Then, it samples the next token  $t_i \sim d_i$  from the distribution  $d_i$  and creates the output sequence  $s_i = s_{i-1} \circ t_i$ , where  $\circ$  denotes the concatenation of a token or sequence with another sequence. Further, if  $t_i = \bot$ , it terminates and returns  $s = s_i$  and, otherwise, it continues to the next step i + 1 in the generation.

Given any prompt sequence, the above autoregressive process determines what (factual) output sequence the LLM generates as a response. However, given a generated output sequence, the above process does not determine what counterfactual output sequence the LLM would have generated if the prompt sequence, or some of the tokens in the output sequence, had been different. To address this limitation, we augment the autoregressive process using a structural causal model (SCM) [15, 16], which we denote as  $\mathcal{M}$ . Our SCM  $\mathcal{M}$ is defined by the following assignments<sup>4</sup>:

$$S_{0} = S_{q}, \quad D_{i} = \begin{cases} f_{D}(S_{i-1}) & \text{if } \texttt{last}(S_{i-1}) \neq \bot, \\ P_{\varnothing} & \text{otherwise} \end{cases}, \quad T_{i} = \begin{cases} f_{T}(D_{i}, U_{i}) & \text{if } D_{i} \neq P_{\varnothing}, \\ \varnothing & \text{otherwise} \end{cases},$$

$$S_{i} = S_{i-1} \circ T_{i} \quad \text{and} \quad S = S_{K},$$

$$(1)$$

where  $S_q$  and  $U = (U_i)_{i \in \{1,...,K\}}$  are independent exogenous random variables, with  $S_q \sim P_Q$  and  $U_i \sim P_U$ , respectively,  $f_D$  and  $f_T$  are given functions,  $P_{\emptyset}$  is the point mass distribution on  $\emptyset$ , and  $last(S_{i-1})$  denotes the last token of the sequence  $S_{i-1}$ . Here, the function  $f_D$  is defined by the transformer architecture of the LLM and the choice of function  $f_T$  and distribution  $P_U$  determines the exact mechanism that the LLM's sampler uses to (stochastically) select the next token  $T_i$ . Note that, there always exists a pair of  $f_T$  and  $P_U$ such that the distribution over tokens  $D_i$  matches the distribution  $P^{\mathcal{M}}(T_i)$  entailed by  $\mathcal{M}$  (see Buesing et al. [48], Lemma 2 for a technical argument). Moreover, note that, in the SCM  $\mathcal{M}$ , the output sequence Scontains the prompt sequence to lighten the notation regarding interventions.

Under this augmented autoregressive process, given an output sequence S = s and noise values U = u, we can generate the counterfactual output sequence the LLM would have generated if the prompt sequence,

 $<sup>^{4}</sup>$ We denote random variables with capital letters and realizations of random variables with lower case letters.

or some of the tokens in the output sequence had been different, deterministically. More formally, given an intervention do $[S_i = \tilde{s}]$ , with  $i \leq |s|$ , the counterfactual output sequence  $S = S_K$  can be computed recursively using the following expression:

$$S_{j} = \begin{cases} s_{j} & \text{if } j < i \\ \tilde{s} & \text{if } j = i \\ S_{j-1} \circ f_{T}(f_{D}(S_{j-1}), u_{j}) & \text{if } j > i \text{ and } \texttt{last}(S_{j-1}) \neq \bot \\ S_{j-1} & \text{otherwise.} \end{cases}$$

$$(2)$$

Note that the key element of this recursive expression for the counterfactual output sequence is the use of the same realized noise values  $u_j$  for  $j \in [K]$  that were used to generate the factual output sequence s. However, without further assumptions, the counterfactual output sequence may be non-identifiable. This is because there may be multiple noise distributions  $P_U$  and functions  $f_T$  under which  $P^{\mathcal{M}}(T_i) = D_i$ , but each pair produces a different counterfactual output sequence—Oberst and Sontag [17] make a similar argument in the context of Markov decision processes. In simpler terms, without explicitly modeling the stochastic mechanism by which the sampler selects the next token in the factual sequence, it is not possible to determine which tokens would have been selected in the counterfactual output sequence. In the next section, we address this issue by focusing on the class of Gumbel-Max SCMs to implement an LLM's sampler.

### 3 Counterfactual Token Generation Using Gumbel-Max SCMs

Under the class of Gumbel-Max SCMs, the function  $f_T$  that implements the sampling of the next token in the SCM  $\mathcal{M}$  adopts the following functional form [17]:

$$f_T(D_i, U_i) = \underset{t \in V}{\operatorname{argmax}} \{ \log D_{i,t} + U_{i,t} \},$$
(3)

where  $U_{i,v} \sim \text{Gumbel}(0, 1)$  are independently distributed Gumbel variables. Importantly, this class of SCMs has been shown to satisfy a desirable counterfactual stability property that can be intuitively expressed as follows. Assume that, at time step *i*, the augmented autoregressive process sampled token  $t_i$  given  $d_i = f_D(s_{i-1})$ . Then, in a counterfactual scenario where  $D_i = d'$ , it is unlikely that, at time step *i*, the augmented autoregressive process would have sampled a token t' other than  $t_i$ —the factual one—unless, under the token distribution d', the relative chance of generating token  $t_i$  decreased compared to other tokens. More formally, for any token distribution  $d' \in \Delta(V)$  with  $d' \neq d_i$  such that

$$\frac{P^{\mathcal{M}}(T_i = t_i \mid D_i = d')}{P^{\mathcal{M}}(T_i = t_i \mid D_i = d_i)} \ge \frac{P^{\mathcal{M}}(T_i = t' \mid D_i = d')}{P^{\mathcal{M}}(T_i = t' \mid D_i = d_i)},$$

it holds that, in the counterfactual scenario where  $D_i = d'$ , the counterfactual token  $T_i \neq t'$ .

In practice, in addition to solving the non-identifiability issues discussed previously, the use of Gumbel-Max SCMs allows for an efficient procedure to sample a sequence of counterfactual tokens with minimal additional memory requirements compared to vanilla token generation. We summarize the procedure in Algorithm 1. Recall that, to generate the counterfactual output sequence, one needs to use the same values  $u_j$  for the noise variables that were used during the factual generation and then perform an autoregressive computation based on Equation 2. Instead of storing the values  $u_j$  for all time steps  $j \in [K]$ , whose dimensionality matches the size of the vocabulary V, Algorithm 1 employs a simple idea: it stores the state of the random number generator  $r_j$  used at each time step  $j \in [K]$  of the factual generation. Then, during the counterfactual generation, it regenerates the values  $u_j = \text{GenGumbel}(r_j)$  on the fly.<sup>5</sup>

<sup>&</sup>lt;sup>5</sup>Storing the realized values of the Gumbel variables requires storing  $\mathcal{O}(KV)$  float values since  $u_j \in \mathbb{R}^V$ . On the other hand, the states of random number generators  $r_j$  take values in  $\mathbb{N}^d$ , where, for instance, d = 16 in pytorch [49]. Thus, our approach requires  $\mathcal{O}(K)$  additional integer memory compared to vanilla token generation.

**ALGORITHM 1:** It returns a counterfactual sequence of tokens using a Gumbel-Max SCM

Input: Random number generator states  $\mathbf{r}$ , factual output sequence s, intervention  $(i, \tilde{s})$ . Output: Counterfactual output sequence s'.

 $\begin{array}{l} \textbf{for } j = 1, \dots, K \ \textbf{do} \\ | \ \textbf{if } j < i \ \textbf{then} \\ | \ s'_j = s_j \\ \textbf{else if } j = i \ \textbf{then} \\ | \ s'_j = \tilde{s} \\ \textbf{else if } j > i \land last(s'_{j-1}) \neq \bot \ \textbf{then} \\ | \ u_j = \text{GenGumbel}(r_j) \\ d'_{j,t} = f_D(s'_{j-1}) \\ t_j = \operatorname{argmax}_{t \in V} \{ \log d'_{j,t} + u_{j,t} \} \\ s'_j = s'_{j-1} \circ t_j \\ \textbf{else} \\ | \ s'_j = s'_{j-1} \\ \textbf{Return } s'_K \end{array}$ 

Remarks on implementation aspects of LLMs. In practice, to avoid sampling tokens with very low probability, LLMs may not directly sample from the distribution over tokens  $d_i$  at each time step i. Instead, a common practice is to sample from a distribution  $\hat{d}_i \in \Delta(V_i)$ , where  $\hat{d}_{i,t} \propto d_{i,t}$  if  $t \in V_i$  and  $\hat{d}_{i,t} = 0$  otherwise, where  $V_i$  is either the set of most likely tokens of size k under  $d_i$ —known as "top-k" sampling—or the set of most likely tokens whose cumulative probability exceeds a given value p under  $d_i$ —known as "top-p" or "nucleus" sampling [14]. We can readily implement top-k sampling and top-p sampling in the SCM  $\mathcal{M}$  by restricting the argmax in Equation 3 to the respective set  $V_i$ . However, in general, the resulting model is not guaranteed to satisfy counterfactual stability.

In all state-of-the-art LLMs, to ensure that the distribution  $d_i$  over tokens at each time step *i* is a valid probability distribution, the final layer in their neural network is a softmax layer. A crucial feature of this layer is the *temperature* parameter,  $\tau$ , which controls the level of uncertainty in  $d_i$ . Intuitively, higher values of  $\tau$  result in a more uniform distribution, while as  $\tau$  approaches zero, the distribution concentrates increasingly on the most probable next token. In the next section, we perform a series of experiments in which we analyze the performance of counterfactual token generation, examining the effects of varying temperature values, as well as the application of top-*k* and top-*p* sampling.

### 4 Experiments

In this section, we experiment with an implementation of our model on Llama 3 8B-instruct [50], a popular open-weights large language model. We start by qualitatively analyzing an example of counterfactual story generation. Next, we quantitatively analyze the similarity between factual and counterfactual text. We conclude with an application of counterfactual token generation in detecting model biases towards demographic groups.<sup>6</sup>

### 4.1 How would the story have unfolded for "Captain Maeve"?

As discussed in Section 3, by using the Gumbel-Max SCM, our approach to counterfactual token generation is guaranteed to satisfy the property of counterfactual stability—counterfactual token generation "prioritizes" selecting the same tokens  $T_i$  that were selected during the factual generation. As a consequence, we expect the counterfactual text generated using counterfactual token generation to be similar to the factual text. Here, we investigate this qualitatively through an anecdotal example of story generation.

<sup>&</sup>lt;sup>6</sup>All experiments ran on an internal cluster of machines, each equipped with 24 Intel(R) Xeon(R) 3GHz CPU cores, 1024GBs of memory and 2 NVIDIA A100 80GB GPUs.

Captain Lyra stood at the helm of her trusty ship, the "Maelstrom's Fury", gazing out at the endless sea. For years, she had sailed the seven seas, seeking the legendary Golden Isle, said to grant a single wish to whoever found it. After a lifetime of searching, Lyra finally spotted the island on the horizon. As she stepped foot on its sandy shores, a warm glow enveloped her. Before her, a chest overflowing with glittering gold and jewels lay at her feet. Lyra's heart soared as she reached for the treasure. But, as she touched the gold, the isle began to fade away, leaving her with nothing but a whispered promise: "The true treasure was the journey, not the gold." Lyra's eyes welled up with tears as she realized the bitter truth — she had sacrificed everything for fleeting riches, and lost the love of her crew, her family, and herself. The "Maelstrom's Fury" sailed away, a lonely shadow on the vast ocean, carrying a captain forever haunted by the what-ifs.

#### (a) Factual story

Captain **Maeve** stood at the helm of her trusty ship, the "Maelstrom's Fury", gazing out at the endless sea. For years, she'd sailed the waves, searching for the fabled Golden Isle, where legend whispered the sea goddess herself granted eternal youth to those who found it. As the sun dipped into the horizon, Maeve spotted it — a shimmering, golden light on the horizon. With a cry of triumph, she steered the ship towards it. As they reached the shore, Maeve leapt out, her eyes drinking in the beauty of the island. And then, she saw her — the goddess, bathing in the golden light. But, as Maeve approached, the goddess vanished, leaving behind a small, intricately carved box. With a heavy heart, Maeve opened it, finding the island's secret: the price of eternal youth was to never find it.

(b) Story generated with interventional token generation, after modifying the protagonist's name

Captain **Maeve** stood at the helm of her trusty ship, the "Maelstrom's Fury", gazing out at the endless sea. For years, she had sailed the seven seas, seeking the legendary Golden Isle, said to grant a single wish to whoever found it. After a lifetime of searching, she finally spotted its shimmering shores. As she stepped onto the island, a radiant light enveloped her, and she wished for her lost love, the brave sailor, Eamon, to return to her. Suddenly, Eamon emerged from the mist, frail but alive. Overjoyed, Maeve scooped him into her arms, and they shared a tender kiss as the sun dipped into the horizon, their love reunited at last.

(c) Story generated with counterfactual token generation, after modifying the protagonist's name

Figure 2: Examples of factual, interventional and counterfactual stories. Panel (a) shows a factual story, as given by the LLM. Panels (b) and (c) show variants of the story resulting from interventional and counterfactual token generation, respectively. In panels (b), (c), we give as input to the LLM the original prompt along with the first sentence of the factual output (non-highlighted text), modified by replacing "Lyra" with "Maeve". Blue (green)-highlighted text indicates the tokens of the output that are identical in the factual story and its interventional (counterfactual) counterpart. Red-highlighted text indicates the differences. In both panels, the temperature parameter is set to  $\tau = 0.9$ .

We use the implementation of our model on Llama 3 8B-instruct with the system prompt "Be creative and keep your response as short as possible." and a query prompt "Tell me a fantasy story about a captain. The story should have either a happy or a sad ending." Figure 2a shows the (factual) generated story about Captain Lyra, her ship the Maelstrom's Fury, and her quest to find a treasure on the Golden Isle. Then, we use the original prompt along with part of the factual output (*i.e.*, the first sentence of the story) as input to the model, modifying the protagonist's name from "Lyra" to "Maeve", and we regenerate the rest of the output using two approaches:

- 1. Interventional token generation: it regenerates the second part of the output using vanilla autoregressive token generation, that is, it samples new noise values  $u_j$  for the second part of the output, as shown in Figure 1c.
- 2. Counterfactual token generation: it regenerates the second part of the output using Algorithm 1, that is, it reuses the same noise values  $u_j$  used in the factual generation for the second part of the output, as shown in Figure 1d.

Figures 2b, 2c present two alternative versions of the factual story generated using the methods mentioned above. These stories reveal several interesting insights. The story generated with interventional token generation starts diverging from the factual story after only a few tokens, as the method lacks memory of the noise values  $u_j$  that resulted in the original output. In contrast, the initial part of the counterfactual output remains identical to the factual output, as expected, due to the counterfactual stability property of the Gumbel-Max SCM and the minor nature of changing the protagonist's name. Although one may expect this



Figure 3: Comparison between interventional and counterfactual token generation. The panels show the edit distance between the factual token sequence and the sequence generated by interventional and counterfactual token generation using (a) the Gumbel-Max SCM defined in Equation 3 and (b) the top-pGumbel-Max SCM and (c) the top-k Gumbel-Max SCM discussed at the end of Section 3, against various values of the temperature parameter  $\tau$ , p and k, respectively. In panels (b, c) the temperature parameter is set to  $\tau = 0.6$ . In all three panels, the edit distance is averaged over 4,000 output sequences, resulting from two independent interventions per factual sequence, and shaded areas represent 95% confidence intervals.

to apply for the rest of the counterfactual output, thinking that the protagonist's name would be irrelevant to the narrative of this particular story, this is not the case. Perhaps surprisingly, the use of "Maeve" instead of "Lyra" results in a partially different output, illustrating that the LLM's probability distributions over next tokens are sensitive even to minor changes. In Appendix A, we also observe differences between the factual and counterfactual outputs resulting from other seemingly irrelevant interventions, such as changing the name of the ship, removing the adjective "trusty" or replacing the word "sea" with "blue".

### 4.2 How similar is counterfactually generated text to the factual one?

In the previous section, we demonstrated through an example that counterfactual token generation results in text that is (partially) similar to the factual text, as expected due to the property of counterfactual stability. Here, we empirically verify this expectation using a quantitative analysis and explore how it is affected by the model parameters.

**Experimental setup.** We first use the implementation of our model on Llama 3 8B-instruct to generate (factual) outputs to 2,000 question prompts sourced from the LMSYS Chat 1M dataset [51]. As a system prompt we use "Keep your replies short and to the point.". Further, for each factual output, we perform two interventions where we replace a randomly selected token  $t_i$  with a token  $t' \neq t_i$ .<sup>7</sup> One of the two interventions restricts the choice of  $t_i$  to the first half of the output sequence and the other restricts it to the second half. Then, for each intervened factual output, we feed the concatenation of the question prompt and the first part of the intervened factual output up to and including token t' as input to our model. We regenerate the second part of the output after token t' using (i) interventional token generation and (ii) counterfactual token generated second part of the output and its factual counterpart using their (normalized) Levenshtein edit distance [52]. In our experiments, we implement our model using the Gumbel-Max SCM defined in Equation 3 as well as the top-p Gumbel-Max SCM and top-k Gumbel-Max SCM discussed at the end of Section 3.

**Results.** Figure 3 summarizes the results, which show that the output sequences generated using counterfactual token generation are more similar to the factual sequences (*i.e.*, the edit distance is lower) than the output sequences generated using interventional token generation. This suggests that, even though the top-p and top-k Gumbel-Max SCMs are not guaranteed to satisfy counterfactual stability, in practice, counterfactual token generation under both models does "prioritize" selecting the same tokens  $T_i$  that were selected during the factual generation.

<sup>&</sup>lt;sup>7</sup>To select t', we set the probability of  $t_i$  in  $d_i$  to 0, re-scale the values of  $d_i$  and use top-p sampling with p = 0.9.



Figure 4: Comparison between factual and counterfactual income, education, and occupation. Panel (a) shows the income of male (female) individuals had they been female (male). Enlarged points correspond to the median income. Panel (b) shows the average difference in the education level of individuals of each race had their race been different. Here, positive values indicate an improvement in education, negative values indicate a decline, and each race is represented with a short description for visibility; refer to Appendix B for further details. Panel (c) shows the distribution shift of occupations among Asian American individuals had they been Black or African American. Green (red) sections indicate the increase (decrease) in the number of Asian American individuals that practice each occupation had they been Black or African American. In all experiments, the temperature parameter is set to  $\tau = 0.8$ .

### 4.3 Does counterfactual token generation reveal model biases?

Common approaches to addressing questions of bias and fairness rely on making counterfactual comparisons based on sensitive attributes [53]. For example, would a person's income have been the same if their race or sex were different? In this section, we focus on a census data generation task, and demonstrate the use of counterfactual token generation to investigate potential biases of the LLM towards demographic groups.

**Experimental setup.** We first use the implementation of our model on Llama 3 8B-instruct to generate (factual) census data. To this end, we use the same input prompt three times with different seeds (see Appendix B for details), requesting 50 individuals each time. The factual data generated by the model consist of 114 fictional individuals including their name, age, sex, citizenship, race, ethnicity, marital status, number of children, occupation, income and education, in this given order. For each fictional person, we consider all possible interventions on each of the sensitive attributes of sex and race. Then, for each intervention, we concatenate the input prompt with the initial part of the output that includes the fictional person's description (up to and including the intervened sensitive attribute). This concatenated input is then used by our model to regenerate the latter part of the output, following the intervention, using counterfactual token generation (*i.e.*, Algorithm 1). Finally, we compare the factual and counterfactual values of attributes such as income, education and occupation.

**Results.** Figure 4 summarizes the results, which reveal several interesting insights. Figure 4a shows that, for most male individuals, their generated income would have decreased had they been female, whereas, for female individuals, it would have sometimes increased and sometimes decreased had they been male. This suggests that the model of the world constructed by the LLM does not only present bias but also exhibits inconsistencies in its perceived relationship between a person's sex and income. Figure 4b shows that, for individuals of all (generated) races, there exists at least one other race that, had they belonged to it, they would have experienced a significant increase or decrease in their education level (refer to Appendix B for the assignment of each education level to a numerical value). Finally, Figure 4c shows that, for Asian American individuals, their occupation would have shifted from STEM to humanities-related occupations had they been Black or African American.

### 5 Conclusions

In this work, we have proposed a causal model of token generation. Using the Gumbel-Max SCM, we have introduced a methodology that enhances state-of-the-art LLMs with the ability to perform counterfactual token generation, allowing them to reason about past alternatives to their own outputs. We have experimentally analyzed the similarity between an LLM's original output and the one generated by counterfactual token generation, and we have demonstrated the use of our methodology in bias detection.

Our work opens many interesting avenues for future work. Our causal model of the autoregressive process underpinning large language models crucially relies on the Gumbel-Max SCM. However, it would be interesting to understand the sensitivity of counterfactual token generation to the specific choice of SCM, and to consider alternative SCMs, especially those that do not satisfy the property of counterfactual stability. Furthermore, we have showcased our model on a single LLM, namely Llama 3 8B-instruct. It would be useful to implement our model on other LLMs and use counterfactual token generation to reveal similarities and differences between the underlying models of the world constructed by different LLMs. Specifically, it would be insightful to see whether the sensitivity of an LLM's counterfactual output changes as its number of parameters increases. Lastly, an interesting future direction would be to explore the use of our methodology in conjunction with human feedback to train (or fine-tune) LLMs that better understand causal relationships.

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## A Additional counterfactual stories

Captain Lyra stood at the helm of her **trusty** ship, the "**Maelstrom's Fury**", gazing out at the endless **sea**. For years, she had sailed the seven seas, seeking the legendary Golden Isle, said to grant a single wish to whoever found it. After a lifetime of searching, Lyra finally spotted the island on the horizon. As she stepped foot on its sandy shores, a warm glow enveloped her. Before her, a chest overflowing with glittering gold and jewels lay at her feet. Lyra's heart soared as she reached for the treasure. But, as she touched the gold, the isle began to fade away, leaving her with nothing but a whispered promise: "The true treasure was the journey, not the gold." Lyra's eyes welled up with tears as she realized the bitter truth — she had sacrificed everything for fleeting riches, and lost the love of her crew, her family, and herself. The "Maelstrom's Fury" sailed away, a lonely shadow on the vast ocean, carrying a captain forever haunted by the what-ifs.

#### (a) Factual story

Captain Lyra stood at the helm of her trusty ship, the "**Cyclone's Rage**", gazing out at the endless sea. For years, she had sailed the seven seas, seeking the legendary Golden Isle, said to grant a single wish to whoever found it. After a lifetime of searching, Lyra finally spotted the island on the horizon. As she stepped foot on its sandy shores, a warm glow enveloped her. Before her, a chest overflowing with glittering gold coins appeared. But, just as she reached for it, a storm brewed, and a rival captain, seeking the treasure for himself, appeared. Lyra fought valiantly, but in the end, she was defeated. As she lay on the beach, her ship destroyed and her crew scattered, Lyra realized her wish had been granted — not for wealth or power, but for the courage to sail through life, no matter the outcome.

(b) Story generated with counterfactual token generation, after modifying the ship's name

Captain Lyra stood at the helm of her trusty ship, the "Maelstrom's Fury", gazing out at the endless **blue**. For years, she'd sailed the seven seas, seeking the legendary Golden Isle, said to grant a single wish to whoever found it. After a lifetime of searching, Lyra finally spotted the island on the horizon. As she anchored the ship and stepped onto the sandy beach, a warm light enveloped her. With trembling hands, she reached out and touched the glittering treasure. The Golden Isle's magic surged through her, and Lyra's greatest desire took hold: to reunite with her lost love, who'd perished at sea many years ago. With tears of joy streaming down her face, Lyra opened her eyes to find her beloved standing before her, alive and well. The two shared a long, tender kiss, surrounded by the sweet scent of tropical flowers. The "Maelstrom's Fury" sailed away, its crew rejoicing, as Lyra and her love disappeared into the sunset, their hearts full of happiness.

(c) Story generated with counterfactual token generation, after changing "sea" to "blue"

Captain Lyra stood at the helm of her \_\_\_\_\_\_ ship, the "Maelstrom's Fury", gazing out at the endless sea. For years, she had sailed the seven seas, seeking the legendary Golden Isle, said to grant a single wish to whoever found it. After a lifetime of searching, Lyra finally spotted the island on the horizon. As she stepped foot on its sandy shores, a warm glow enveloped her. Before her, a chest overflowing with glittering gold and jewels lay at her feet. Lyra's heart soared as she reached for the treasure. But, as she touched the gold, the isle began to fade away, leaving her with nothing but a whispered promise: "The true treasure was the journey, not the gold." Lyra's eyes welled up with tears as she realized the bitter truth — she had sacrificed everything for fleeting riches, and lost the love of her crew, her family, and herself. The "Maelstrom's Fury" sailed away, a lonely shadow on the vast ocean, carrying a captain forever lost at sea.

(d) Story generated with counterfactual token generation, after deleting the word "trusty"

Figure 5: Comparison between the factual story and counterfactual variants. Panel (a) shows the same factual story as in Section 4.1. Panels (b, c, d) show the story resulting from various interventions. In each case, the first sentence (non-highlighted text) is provided as input to the LLM, with the word(s) in bold (or left empty) representing the intervention. The remainder of the output is regenerated using counterfactual token generation. Text highlighted in green indicates the tokens of the output that are identical in the factual story and its counterfactual counterpart. Red-highlighted text indicates the differences. In all panels, the temperature parameter is set to  $\tau = 0.9$ .

System: Return only the following information: Name, Age, Sex, Citizenship, Race, Ethnicity, Marital Status, Number of Children, Occupation, Income, Education. For Race, choose only between following options: White American, Black or African American, American Indian or Alaska Native, Asian American, Native Hawaiian or Other Pacific Islander, Other or Two or more races (multiracial). For Ethnicity, choose only between following options: Non-Hispanic/Latino or Hispanic/Latino. Return a list in json format delimited by "```."

User: Generate census data of 50 fictional people.

Figure 6: The prompt used for census data generation.

## **B** Additional details on the experimental setup of Section 4.3

In this section, we provide additional details about the census generation experiment discussed in Section 4.3. Figure 6 shows the complete system and user prompts used to generate the census data. For race and ethnicity, we instructed our model, through the system prompt, to select values among those reported in the latest (2020) US Census. We used this prompt three times with different seeds. Despite our request for 50 individuals per generation, the LLM only generated 34, 39 and 41 individuals each time, resulting in a total of 114 individuals. Table 1 contains the full descriptions of the race attribute values, of which shortened versions were used in Figure 4b. Finally, Table 2 lists the numerical values assigned to the (categorical) education attribute values, used to compute the difference in education level shown in Figure 4b.

Table 1:	Short	and	full	descri	ption	of	all	races

Short	Full
Native	American Indian or Alaska Native
Asian	Asian American
African	Black or African American
Hawaiian	Native Hawaiian or Other Pacific Islander
Other/2+	Other or Two or more races (multiracial)
White	White American

Table 2: Numerical value assigned to each (categorical) value of the education attribute

Education	Numerical Value
High School Diploma	1
High school diploma	1
Associate's degree	2
Some college	2
Bachelor's degree	3
Master's degree	4
Ph.D.	5
Law Degree	5
Law degree	5
Juris Doctor	5
Medical Degree	5
Medical degree	5
Dental degree	5
Dentistry degree	5