# **Can One Token Make All the Difference? Forking Paths in Autoregressive Text Generation**

Eric Bigelow<sup>1, 2</sup>, Ari Holtzman<sup>3</sup>, Hidenori Tanaka<sup>\*1, 2</sup>, and Tomer Ullman<sup>\*1</sup>

<sup>1</sup>Harvard University, <sup>2</sup>NTT Research, <sup>3</sup>University of Chicago

**Background** Large Language Models (LLMs) are often treated as black boxes with mysterious capabilities that emerge during next-word prediction, and a good deal of current research is devoted to interpreting and understanding LLM text generation behavior. One way to assess a black box system is to consider what possible things it *could* have done, but didn't. In text generation, we can liken the a text sequence to a path the system took through semantic space, and ask: what other paths could the system have taken? Are there key forking points where re-sampling the system at that specific token, but not others, would lead to very different paths? We propose a novel methodology for answering these questions with what we call Forking Paths Analysis (Borges, 1941).

The most common method for estimating uncertainty in LLMs is to sample a single text output, and inspect logit probabilities for the final answer token (e.g. p("Yes") or p("No") given 'So, the answer is ") (Kadavath et al., 2022; Hu and Levy, 2023). A less common approach is to sample a batch of output texts using stochastic decoding, and compute a histogram over final answers (Wang et al., 2023; Xiong et al., 2023). However, the first method does not explain how an LLM can generate two distinct solution attempts for a problem. The uncertainty will not be reflected in the last token of each output, since that token will be deterministic given the proof preceding it. The second method explains uncertainty in the final answer, but ignores the rest of the text preceding the answer. For many LLM uses, such as proving a theorem, the steps leading to the final answer can be as important as the answer itself. By contrast, our Forking Paths Analysis considers both individual token sequences as well as final outcome distributions. This method offers a detailed view into the uncertainty dynamics underlying each step of text generation, and enables us to test the hypothesis that individual tokens are

pivotal in that re-sampling at specific points can send text generation in a very different direction. Our Forking Paths Analysis does not require access to an LLM's internal activations, and relies only on logit probabilities available in some black-box LLM APIs (also see Morris et al. (2023)).

**Our primary contributions:** (a) a novel method, Forking Paths Analysis, for understanding uncertainty in text generation by representing it as multivariate time series aggregated over many samples, and by (b) applying change point detection models to statistically test the hypothesis that there are sharp change points in text generation; (c) we use Forking Paths Analysis to demonstrate striking dynamics in text generation, including significant change points where a single token dramatically affects subsequent text.



Figure 1: Forking Paths Analysis in three parts (Part 1, Top) Given a single text completion  $x^*$  and top-k alternate tokens at each step t, we re-sample S completions  $x_{>t}^{(s)}$  and extract <u>outcome vector representations</u>  $\underline{R(x)}$  for each sample. (Part 2, Middle) We aggregate extracted outcomes as weighted distributions, equivalent to a multivariate time series  $o_t(x^*)$ . (Part 3, Bottom) We convert the distributions into a univariate series using a semantic drift transformation, and apply a Change Point Detection model to identify sudden changes.



Figure 2: Forking Paths Analysis applied to a math word problem (Top) Outcome distribution  $o_t$  for GSM8k grade school math question 97. Final answer probabilities are plotted as different colors. Outcomes outside the top-5 answers are grouped into *Other*. Correct answer: 70. (Middle) Semantic drift transformation  $y_t = d(o_0, o_t)$ , and (Bottom) change point detection posterior probability  $p(\tau = t)$  at each step t.

**Methods** Conditional re-sampling (Fig. 1, Part 1) proceeds in three stages: (1) sample a base text sequence  $x^*$  and collect token logit probabilities  $p(x_t = w | x_{< t}^*)$  for the top-k tokens w at each index t, (2) for each index t and each alternate token w where  $p(x_t = w | x_{< t}^*) > \epsilon$  is greater than some threshold  $\epsilon$ , draw S samples of alternative text completions  $x_{>t}^{(s)} LLM(x_{< t}^*, x_t = w)$ , (3) for all completions concatenated with their input text, extract an outcome representation  $R(x_{< t}^*, x_t = w, x_{>t}^{(s)})$ , where R may be a one-hot embedding for the final answer extracted using another LLM, or R may be a semantic embedding vector.

We define *outcome distributions*  $o_t$  for individual token indexes t as weighted vector representations:  $o_t(x^*) = \mathbb{E}_{w,s} \left[ R(x^*_{< t}, x_t = w, x^{(s)}_{>t}) \right]$ 

In the tasks shown here, R(x) is a one-hot encoding of the answer in x (e.g. 'A', 'B', 'C', 'D'), extracted using a secondary LLM with a prompt template. In future work, we will explore openended text generation tasks where R(x) is instead a dense vector embedding of x.

We use  $o_t$  to test the hypothesis that there are specific change points t where text generation shifts suddenly. First, we convert  $o_t$  into a univariate time series for tractable multiple Change Point Detection (CPD) (Fearnhead, 2006) using a *semantic drift* metric (Kulkarni et al., 2015). Each point in the shift series  $y_t = d(o_0, o_t)$  is the distance between the initial outcome distribution  $o_0$  and subsequent time steps  $o_t$ , given a distance metric d. We then run Bayesian CPD (Zhao et al., 2019) to identify change points  $\tau$  by fitting separate regression models to each segment  $y_{\tau_i,...,\tau_{i+1}}$ .

Domain	Task	1+ Changes
Symb. Reasoning	CoinFlip	0%
	LastLetter	71%
Math Reasoning	AQuA	14%
	GSM8k	20%
Complex Q.A.	MMLU	0%
	HotpotQA	40%
Story Generation	StoryCloze	14%

Table 1: Change Point Detection results for each task We use 7 tasks commonly used for LLM evaluation. The right-most column lists % of question time series for which our Change Point Detection model assigns at least 90% probability to there being  $\geq 1$  change points.

**Experiments** We present preliminary results for experiments on gpt-3.5-turbo-instruct-0914 using 7 datasets used for evaluating LLMs across a wide range of domains: Symbolic Reasoning (Wei et al., 2022), Math. Reasoning (Ling et al., 2017; Cobbe et al., 2021), Complex Question Answering (Hendrycks et al., 2020; Yang et al., 2018), and Story Generation (Mostafazadeh et al., 2017)<sup>1</sup>. For the first 6 tasks, we add a zero-shot CoT prompt (Kojima et al., 2022).  $x^*$  is greedily decoded. We show results for 5 – 15 prompts for each of 7 tasks (*S*=30,  $\epsilon$ =.05), and soon will have results for 100 prompts each. Note each question in our dataset aggregates over millions of sampled tokens.

In many  $o_t$ , we observe dramatic non-linear uncertainty dynamics over the course of text generation. In time series such as AQuA-60927, we see a pattern where the LLM is equally uncertain across answers until one token is generated. In others such as HotpotQA-79442 and LastLetter-342, we see patterns where one stable regime of certainty maintains for dozens or hundreds of tokens, before shifting to another stable regime, and then a third or fourth regime (see App. B). These dynamics may suggest in-context model selection (Bigelow et al., 2024). In many time series, particularly in CoinFlip and StoryCloze, we see minimal uncertainty with no obvious change points. We find more change points in some tasks than others (Table 1).

The rich token-level uncertainty dynamics we see in our Forking Paths Analysis show us how black-box LLMs can 'fork' during text generation and transition suddenly from one pattern to something quite different. At the edge of this transition, even a single token can make all the difference.

<sup>&</sup>lt;sup>1</sup>We alter StoryCloze to instead request short stories beginning with 1 specified sentence and ending with 1 of 2 equally plausible final sentences.

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# **Appendices**

# **A** Estimating Outcome Distributions



Figure 3: Outcome distributions  $o_t$ ,  $o_{t,w}$  are computed as a weighted average of vector representation Racross sampled completions and, in the case of  $o_t$ , across alternate tokens w.

To compute outcome representations, we aggregate samples into distributions - weighted vector representations – over token indexes  $(o_t)$  and alternate tokens  $(o_{t,w})$ :

$$o_{t,w}(x^*) = \mathbb{E}_s \left[ R(x^*_{t}) \right]$$

$$o_t(x^*) = \mathbb{E}_w \left[ o_{t,w}(x^*) \right]$$

$$= \sum_w p(x_t = w \mid x^*_{t} \mid x^*_{t})$$

$$putcome Distr. Next-Word Prediction Sample Probability Outcome Representation$$

Outcome Distr.

Sample Probability

Outcome Representation

After de-duplicating samples, we weight by (a) the average next-token probability for sampled completions, normalized by number of tokens T in sample  $x_{>t}^{(s)}$ :

$$p(x_{>t}^{(s)}|x_{$$

as well as (b) single next-token probability for alternate tokens  $p(x_t = w | x_{<t}^*)$  (Fig. 3).

Note that  $o_t$  is the main subject of this work, but we also use  $o_{t,w}$  for an alternate Forking Tokens Analysis approach in App. C.

### **B** Additional Examples

Below, we show a Forking Paths Analysis (FPA) for one example each of all 7 of our datasets. The first 5 examples are hand picked to show change points. However, these 5 examples are taken from a relatively small sample (5-15 questions per task) which includes other change point FPA results not shown here.

Examples for the first 5 datasets – GSM8k (Fig. 4), AQuA (Fig. 5), LastLetter (Fig. 6), MMLU (Fig. 7), and HotpotQA (Fig. 8) – show dramatic uncertainty dynamics in  $o_t$  with change points in  $y_t$ . Note that for text examples in this section, quotes are shown from the model responses (highlighted text in each Figure), and we <u>underline</u> the a single words with high change point probability (dark red in subfigure (b) of each figure) according to our Change Point Detection model.

For the AQuA and LastLetter examples, we see a pattern of stable uncertainty for a long period, followed by a sudden collapse into high certainty. Note that for LastLetter, the high probability on Other is the amount of probability mass unassigned across tokens with less than  $\epsilon$  next-word probability. In the case of AQuA-60927, this collapse to B (green; also the correct answer) occurs when a key token in the final answer is sampled – the first digit of \$4,500. In the case of LastLetter-342, the second mode collapse occurs when sampling tokens in the final answer nlyhth. However, the first change in LastLetter-342 follows a different pattern, instead moving from a moderately high certainty regime to very low certainty. This change occurs when two seemingly innocuous return symbols ... Elisabeth".split()  $n \cong n$  Next, we need ... are generated. The distribution suddenly shifts from  $\sim 50\%$  confidence in *olah* (the correct answer) to low certainty across answers (blue area in Fig. 6).

We see additional change points and sudden transitions between stable regimes in the examples for GSM8k, MMLU, and HotpotQA. In **GSM8k-97** (Fig. 4) we see the correct answer 70 (brown) hold 20 - 30% of the overall probability mass for a few dozen tokens, before suddenly disappearing after 2x = 40 is sampled, being replaced by the answer 54 (purple). Eventually  $\ln \ln Now$ , we can is sampled and this answer disappears as the LLM collapses into full certainty of 46 (red). The change point at 2x = 40 might be expected since this token is key in articulating a certain chain of reasoning. However, the token at n n Now, we can is more surprising.

In MMLU and HotpotQA examples, we see regimes of stable outcome distributions that suddenly collapse to high certainty in a single answer. For MMLU-32, this occurs at a perhaps surprising time, after the word scenario is generated in as of 2020. In scenario 2, the main character. In HotpotQA-79442 we see a striking pattern where the correct answer Peter Noone is at first the dominant response (red area). First it seems to gradually drift towards the alternate response, Eddie Vedder (orange), but then at two points it sharply jumps. The first of these tokens is surprising, in a relatively inert seeming down, whereas the second change point is a token in the final answer: Both musicians have had successful careers in the music indus*try, but which one also became an actor?*\*n* \*n The* answer is Eddie Vedder.

Finally **CoinFlip-61** and **StoryCloze-274** show example time series with no significant forking points. Time series such as these help us benchmark our Change Points Detection model, since we expect there to be no change points in these series

One common theme of our observed change points is that some are at times we might expect, key meaningful words which distinguish between chains of reasoning or themes in text generation. Other change points are at times we might not expect, seemingly innocuous words such as Now or minor tokens such as punctuation and escape characters \n \n. Tokens such as this may relate to distinctions between surface and content forms (Holtzman et al., 2021), vaguely analogous to syntax (surface form) and semantics (content) in natural language. Following this intuition, \$4,500 or 2x = 40 may be examples of 'content' token that clearly distinguishes between multiple underlying content forms, whereas ... *Elisabeth*".*split(*) n ``  $n \in Next$ , we need ... and  $n \in Now$ , we can are examples where a 'surface' token is distinguishing between latent content forms.



(a) GSM8k question 97

 $o_t$  outcome distribution, drift  $y_t$ , and change point probability  $p(\tau = t)$ 

Question: Janet is collecting the results of Herbert Hoover Elementary School's annual standardized test. 340 out of 500 third-graders passed, along with 40 out of 100 fourth grades? The 400 fifth graders had a pass rate that was twice the fourth grades? pass rate. What is the school's overall pass rate? Answer:	First, we need to find the total number of students who passed, but wis to tail of show that 34 which regulates and 40 bourth grades passed, so that's as total of 340 + 40 = 380 students, inn'Next, we need to find the pass rate for the fifth grades. We are tool that their pass rate was to text the fourth gradery pass rate, so we can set up the equation $y = 40$ , where x represents the fourth gradery pass rate: Solving for x, we get x = 0. This means that the fifth gradery pass rate was 20% in both we get x = 0. This means that the fifth gradery pass rate was 20% in both we get x = 0. This means that the fifth gradery pass rate was 20% in both we get x = 0. This gradery was passed by multiplying the total number of fifth graders who passed in particle was 20% in both we get x = 0. This graders who passed, in particle was a straight and the total number of fifth graders who passed in the straight and the straight and the straight and the straight and the particle was passed by multiplying be total number of fifth graders who passed in the straight and the straight and the straight and the straight and the straight and the straig	<b>1996.</b> we need to find the total number of students who passed the test <b>We</b> movi that 340 third graders and 40 fourth graders passed, solutily is total of $340 \pm 40 = 380$ students jum Next, we need to find the pass rate for the find graders. We grad to that their pass rate was twice the fourth graders' pass rate lower can set up the equation $2x = 40$ , where a represent the fourth graders' pass rate. Solving for $x$ , we get $x = 20$ . This means had the fifth graders' pass rate was 200 min Now, we can find the iotal number of fifth graders' pass rate (was 200 min Now, we can find the iotal number of fifth graders' pass rate (was 200 min Now, we can find the iotal number of fifth graders' pass rate (was 200 min Now, we can find the row of fifth graders who passed i up first pass rate (200 min Now).
Answer: .et's think step by step.	students who passed from each grade $(380 + 80 = 460)$ and dividing by the total number of students $(500 + 100 + 400 = 1000)$ . This gives us an overall pass rate of 460(1000 = 46%) hybrefore, the overall pass rate for Herbert	the pass rate (20%). This gives us 400 x 0.20 = 80 fifth graders who passed. whoFinally, we can find the overall pass rate by adding the number of students who passed from each oracle [380 + 80 = 460) and dividing by the
	Hoover Elementary School's annual standardized test is 46%.	total number of students (500 + 100 + 400 = 1000). This gives us an overall pass rate of 460/1000 = 46%. \n\n Therefore, the overall pass rate for Herbert Hoover Elementary Schools annual standardized test is 46%.
	(c) Change point detection probabili-	
	$A^{*}$ $A^{*}$ $A^{*}$ $B^{*}$ $B^{*$	

(b) Prompt: GSM8k question 97

ties  $p(\tau = t)$ . Red is high probability, (d) Token logit probabilities. Red is yellow is low.



low probability, yellow is high.



(a) AQuA question 60927

 $o_t$  outcome distribution, drift  $y_t$ , and change point probability  $p(\tau = t)$ 



Figure 5:



(a) LastLetter question 342  $o_t$  outcome distribution, drift  $y_t$ , and change point probability  $p(\tau = t)$ 

	This, we need to separate the words in the given string, we can do this by	
	using the split() method, which will create a list of words.\n\n```\nwords =	
	"Lino Mariel Aditya Elisabeth".split()\n` \nmNext, we need to access the last	First, we need to separate the words in the given string. We can do this by
	letter of each word. We can do this by using the index -1, which will give us	using the split() method, which will create a list of words.\n\n" \nwords =
Question:	the last element of the list.\n\n```nlast_letters = [word[-1] for word in words]	"Lino Mariel Aditya Elisabeth".split()\n" \n\nNext, we need to access the last
Take the last letter of each word in "Lino Mariel Aditya Elisabeth" and	\n```\n\nNow, we have a list of the last letters of each word. We can use the	letter of each word. We can do this by using the index -1, which will give us
concatenate them.	join() method to concatenate them into a single string.\n\n``\nconcatenated =	the last element of the list.\n\n""\nlast_letters = [word[-1] for word in words]
	".join(last_letters)\n```\n\nFinally, we can print the result.	\n```\n\nNow, we have a list of the last letters of each word. We can use the
Answer:	\n\n```\nprint(concatenated)\n```\n\nThe output will be:	join() method to concatenate them into a single string.\n\n```\nconcatenated =
Let's think step by step.	\n\n``\nnlyhan\n```\n\nSo, the final code will be:\n\n```\nwords = "Lino	"".join(last_letters)\n``\n\nFinally, we can print the result.
	Mariel Aditya Elisabeth".split()\nlast_letters = [word[-1] for word in words]	\n\n```nprint(concatenated)\n```\n\nThe output will be
	\nconcatenated = "".join(last_letters)\nprint(concatenated)\n```	\n\n```\nnlyhth\n```\n\nSo, the final code will be:\n\n```\nwords = "Lino
		Mariel Aditya Elisabeth".split()\nlast_letters = [word[-1] for word in words]
		\nconcatenated = "".join(last_letters)\nprint(concatenated)\n

(c) Change point detection probabilities  $p(\tau = t)$ . Red is high probability, yellow is low.

(d) Token logit probabilities. Red is low probability, yellow is high.

Figure 6:

(b) Prompt: LastLetter question 342







Question: For which of these two scenarios does the main character (who uses I/me/my) do something clearly morally wrong, according to ordinary moral standards in the US as of 2020? Scenario 1 | toopped by and guewer my gittfriend some flowers before driving home to my wife. Scenario 2 | I copied and pasted so I could write my paper with sources found on the internet.

Choices: A) Wrong, Wrong B) Wrong, Not wrong C) Not wrong, Wrong D) Not wrong, Not wrong

Answer: Let's think step by step.

(b) Prompt: MMLU question 32

(c) Change point detection probabilities  $p(\tau = t)$ . Red is high probability, (d) yellow is low.

(d) Token logit probabilities. Red is low probability, yellow is high.

Figure 7:



(c) Change point detection probabilities  $p(\tau = t)$ . Red is high probability, yellow is low.

(b) Prompt: HotpotQA question 79442 yellow is

Figure 8:



(a) CoinFlip question 61

 $o_t$  outcome distribution, drift  $y_t$ , and change point probability  $p(\tau = t)$ 



Question: Q: A coin is heads up. Mateah flips the coin over. Hallsten flips the coin over. Is the coin still heads up?

(b) Prompt: CoinFlip question 61

Answer: Let's think step by step.

> (c) Change point detection probabilities  $p(\tau = t)$ . Red is high probability, (d) Token logi yellow is low. low probability

(d) Token logit probabilities. Red is low probability, yellow is high.

(d) Token logit probabilities. Red is

low probability, yellow is high.

Figure 9:



(a) StoryCloze (2 Choice) question 274  $o_t$  outcome distribution, drift  $y_t$ , and change point probability  $p(\tau = t)$ 



question 274

Figure 10:

low probability, yellow is high.

## C Forking Tokens Analysis

Our Forking Tokens Analysis (FTA) considers  $o_{t,w}$  rather than  $o_t$ , as in our Forking Paths Analysis (FPA). Fig. 11 offers a visual intuition for  $o_{t,w}$  and how individual tokens w can fork, in addition to token indexes t as in FPA.

For this, we consider whether, for a given token index t, alternate tokens w being sampled cause the outcome distribution  $o_{t,w}$  to deviate from the greedy outcome distribution  $o_{t,w^*}$  by at least some threshold  $\varepsilon$ . Following this, we define the *forking survival function* S(t) as the probability that, across t, text generation 'survives' forking from  $o_{t,w^*}$  to a very different outcome distribution  $o_{t,w}$ :

$$S(t) = 1 - \prod_{t'=1}^{t} \mathbb{E}_{w} \left[ o_{t',w} \not\approx o_{t',w^{*}} \right]$$
  
=  $1 - \prod_{t'=1}^{t} \sum_{w} p(x_{t'} = w | x^{*}_{< t'}) \mathbb{1} \left[ d(o_{t',w}, o_{t',w^{*}}) > \varepsilon \right]$ 

This is loosely analogous to our semantic drift transformation  $y_t = d(o_0, o_t)$  in FPA, where  $o_0$  was the base distribution and  $o_t$  was the alternative when computing  $y_t$ . In FTA, instead we have  $o_{t,w^*}$  as the base and  $o_{t,w}$  as the alternative.

In Fig. 12 we see that survival rate for this sequence goes to 0 over even very high thresholds – Note that a distance of  $\varepsilon = .7$  for  $L_1$  distance d is very high since vectors  $o_{t,w^*}$  and  $o_{t+1,w}$ ) are normalized to sum to 1.



Figure 11: Forking Token outcome distributions  $o_{t,w}$  These sankey plots (or parallel sets plots) show  $o_{t,w}$  across w, for 4 different values of t. Each outcome, in this case a final answer (e.g. *OLAH* or *NLYHTH*), is colored differently, and the colored bars on the left and right side of each sankey show how one token's outcome distribution  $o_{t+1,w}$  can change significantly from the previous time's outcome distribution  $o_{t+1,w^*}$ . Here, we see  $o_{t,w}$  for 4 values of t in LastLetter-342, around the second transition in this examples analysis (see Fig. 6 in App. B). At this transition, the tokens explicitly state the final answer, and so it's not surprising that we see a transition here. At the third time step t, we see that different tokens lead to completely different outcome distributions.



Figure 12: Forking Token Survival Analysis Here we show the forking token survival rate S(t) (Bottom) for different distance thresholds of  $\varepsilon$ , where (Middle) shows the forking probability  $\sum_{w} p(x_{t'} = w | x_{<t'}^*) \mathbb{1} \left[ d(o_{t',w}, o_{t',w^*} at each t, and (Top) shows baselines of the token-by-token logit probabilities (pink dotted; re-normalized from range <math>[0, 1]$  to [0, 5]) and the number  $|tokens_t|$  of alternate tokens w at step t (brown). Results shown for LastLetter-342 (also see Fig. 6 in App. B).