

# Token Embeddings Violate the Manifold Hypothesis

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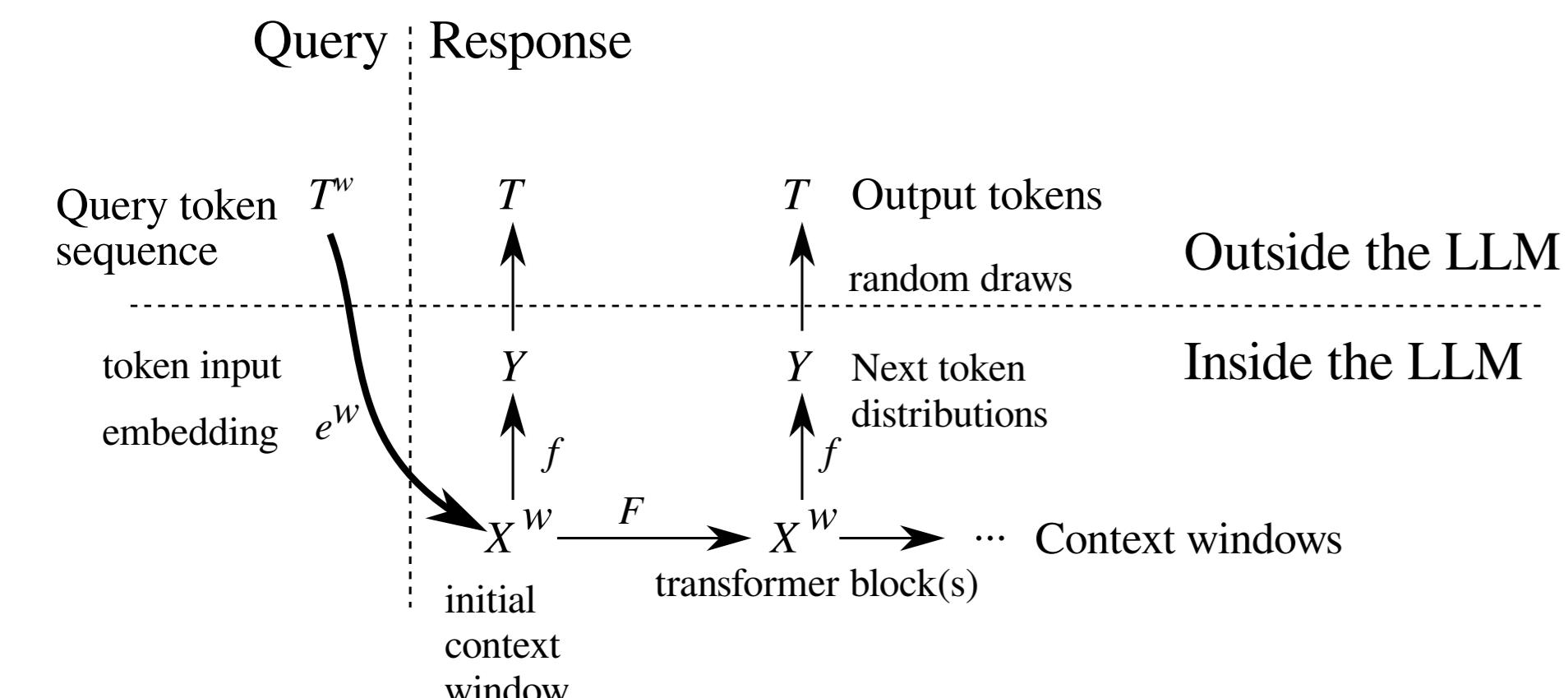


## The manifold and fiber bundle hypotheses

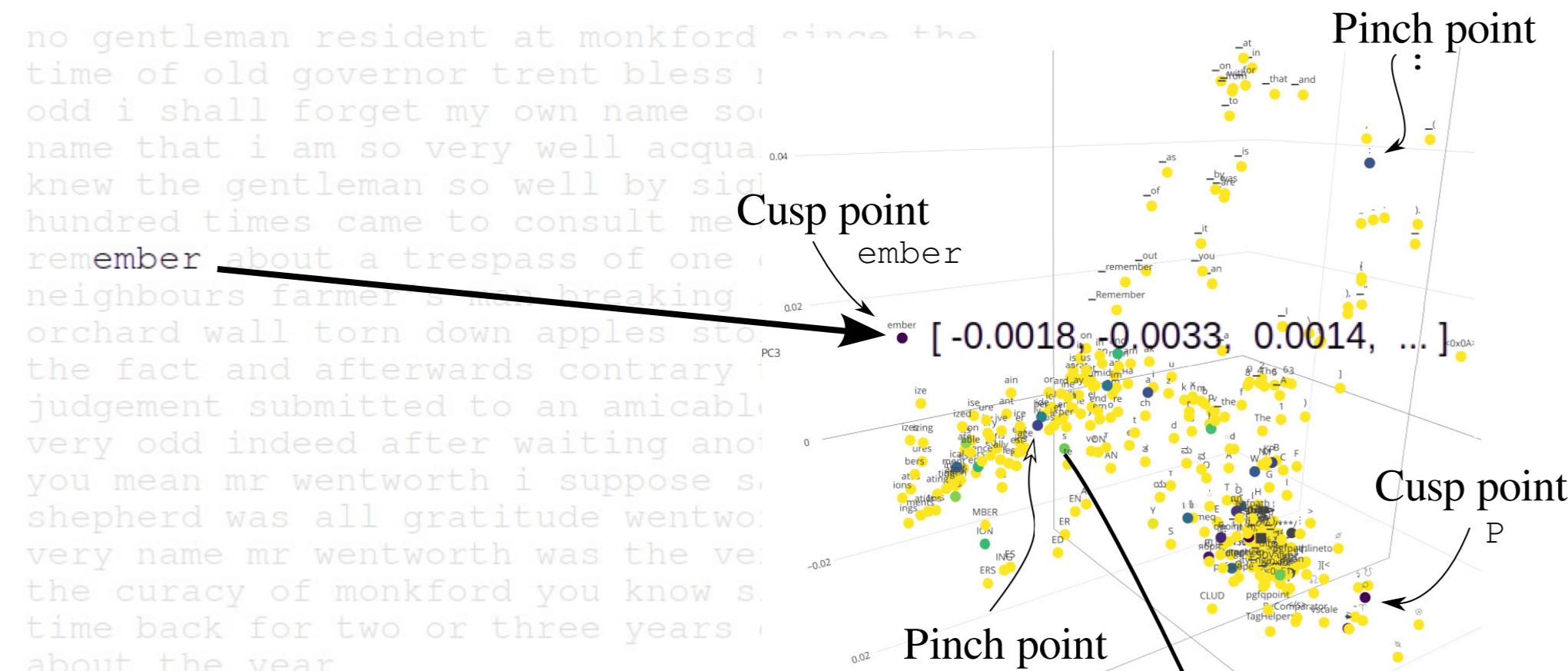
Hypotheses we test. We assume the token subspace has reach  $\tau > 0$ , and estimate the dimension in the ball centered at token  $\psi$  with radius  $r < \tau$ .

	Manifold test	Fiber bundle test
$H_0$	There is a unique dimension at $\psi$	The dimension at $\psi$ in a ball of radius $r$ does not increase as $r$ increases.
$H_1$	There is not a unique dimension at $\psi$	The dimension at $\psi$ increases at some $r$

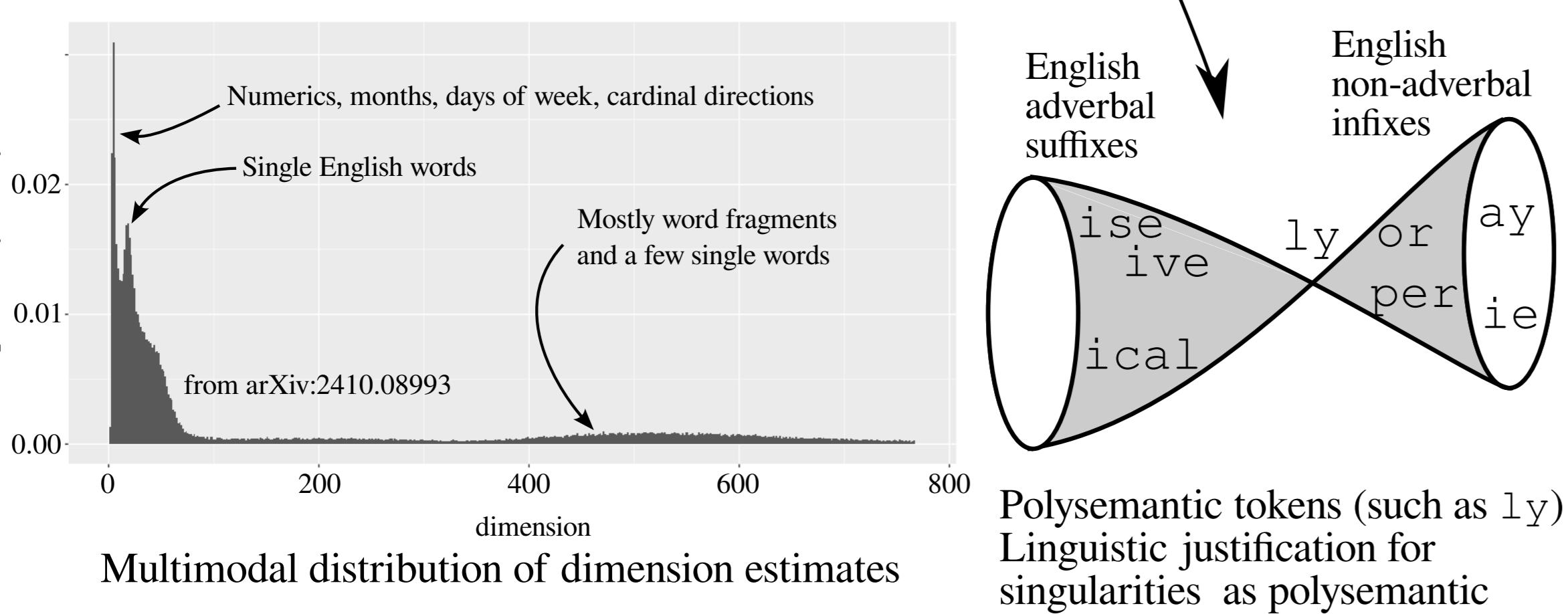
## Token embeddings for LLMs



PCA plot of first 3 principal components of Mistral7B



## Evidence against the manifold hypothesis



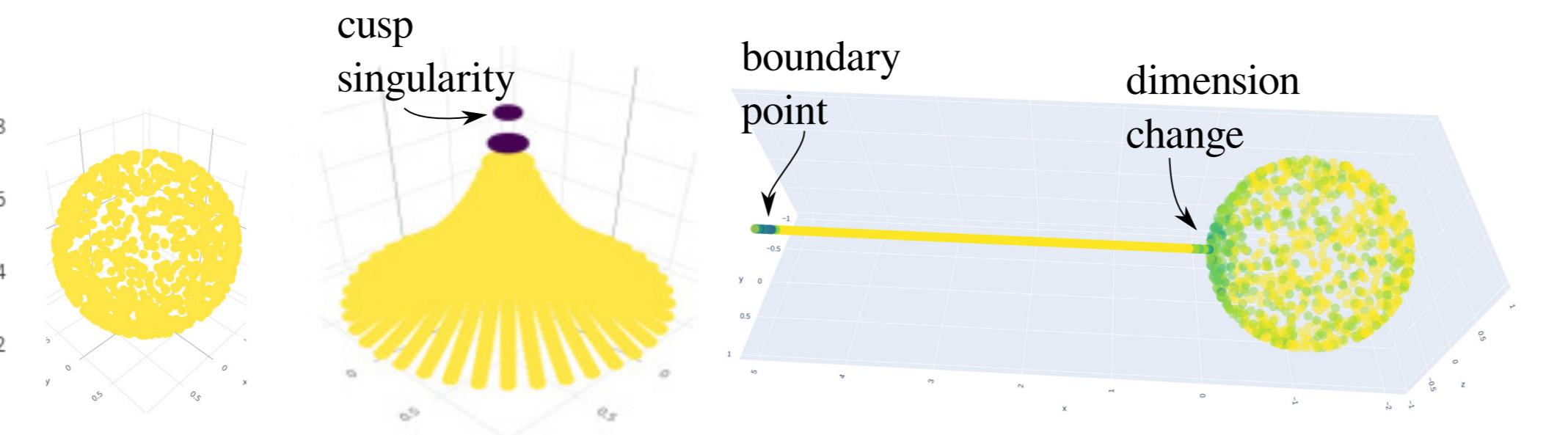
## Implementing our tests

### Algorithm 1 Manifold and fiber bundle tests

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Require:  $x_1, \dots, x_n \in \mathbb{R}^\ell$ : coordinates for each point
Require:  $v_{min}$  and  $v_{max}$ : minimum and maximum number of tokens in neighborhood
Require:  $W$ : sliding window size
Require:  $\alpha$ : significance level
Ensure:  $p_1$ : set of  $p$  values for manifold hypothesis
Ensure:  $p_2$ : set of  $p$  values for fiber bundle hypothesis
Ensure: Set of dimension estimates
1: procedure MANIFOLDANDFIBERBUNDLETEST( $x_\bullet, v_{min}, v_{max}, W$ )
2:   Compute  $n \times n$  pairwise distance matrix  $D$  between all tokens
3:   for Each column of  $D$  do ▷ Columns correspond to token indices
4:     Sort the column ▷ Now row indices of distance matrix are volumes, entries are radii
5:     Retain rows  $v_{min}$  through  $v_{max}$ 
6:     Compute log-log slopes (= dimension estimates) along the column
7:   end for ▷ Run two sample  $T$ -test along adjacent sliding windows of size  $W$  with level  $\alpha$ :
Manifold test: Append to  $p_1$ : the  $p$ -value for the hypothesis that the slope is constant
Fiber bundle test: Append to  $p_2$ : the  $p$ -value for the hypothesis that the slope decreases with row index
8:   Store both  $p$  values and slope with corresponding token (column index)
9: end for
10:  Apply Holm-Bonferroni multiple test correction to both sets of  $p$ -values
11: end procedure

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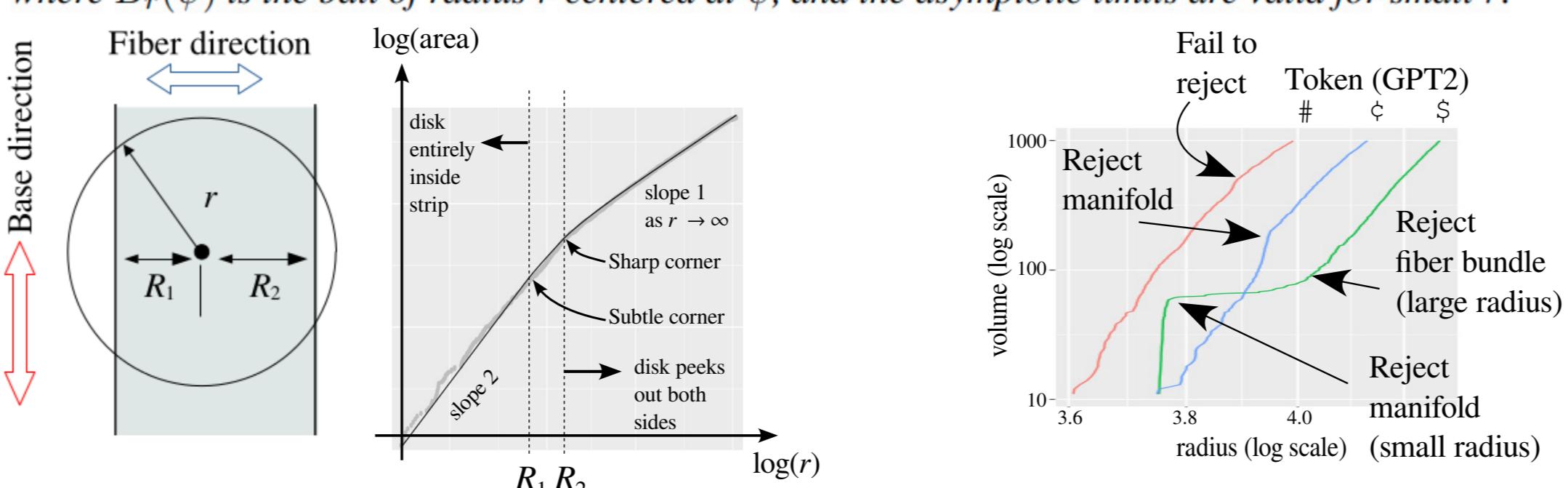


## Theoretical justification

**Theorem 1.** Suppose that  $T$  is a compact, finite-dimensional Riemannian manifold with boundary, with a volume form  $v$  satisfying  $v(T) < \infty$ , and let  $p : T \rightarrow S$  be a fiber bundle. If  $e : T \rightarrow \mathbb{R}^\ell$  is a smooth embedding with reach  $\tau$ , then there is a function  $\rho : e(T) \rightarrow [0, \tau]$  such that if  $\psi \in e(T)$ , the induced volume  $(e_*v)$  in  $\mathbb{R}^\ell$  satisfies

$$(e_*v)(B_r(\psi)) = \begin{cases} O(r^{\dim T}) & \text{if } 0 \leq r \leq \rho(\psi), \\ (e_*v)(B_{\rho(\psi)}(\psi)) + O((r - \rho(\psi))^{\dim S}) & \text{if } \rho(\psi) \leq r, \end{cases}$$

where  $B_r(\psi)$  is the ball of radius  $r$  centered at  $\psi$ , and the asymptotic limits are valid for small  $r$ .



**Theorem 2.** Let  $Z$  be a  $d$ -dimensional bounding manifold for the token subspace, such that  $T \subseteq Z$ . Consider an LLM with a context window of size  $w$ , in which the latent space of tokens is  $\mathbb{R}^\ell$ , and we collect  $m$  tokens as output from this LLM.

Suppose the following, (enough tokens are collected from the response)  $m > \frac{2wd}{\ell}$ , but (the context window is longer than the number of tokens we collected)  $w \geq m$ . Under these conditions, a generic set of transformers yields a topological embedding of  $T^w = T \times \dots \times T$  into the output of the LLM.

## Experimental results

Running the two hypothesis tests on four open weight LLMs

Model	Manifold rejects	Fiber bundle		
		Smaller Radius dim.	rejects	Larger radius dim.
GPT2 $n = 50257$	66 $p \approx 3 \times 10^{-8}$	Q1: 20 Q2: 389 Q3: 531	12 $p \approx 9 \times 10^{-6}$	Q1: 8 Q2: 14 Q3: 32 $p \approx 3 \times 10^{-8}$
Llemma7B $n = 32016$	33 $p \approx 5 \times 10^{-9}$	Q1: 4096 Q2: 4096 Q3: 4096	0 N/A	Q1: 8 Q2: 11 Q3: 14 $p \approx 3 \times 10^{-4}$
Mistral7B $n = 32016$	40 $p \approx 3 \times 10^{-7}$	Q1: 9 Q2: 48 Q3: 220	1 $p \approx 8 \times 10^{-4}$	Q1: 5 Q2: 6 Q3: 9 $p \approx 8 \times 10^{-5}$
Pythia6.9B $n = 50254$	54 $p \approx 2 \times 10^{-7}$	Q1: 2 Q2: 108 Q3: 235	0 N/A	Q1: 2 Q2: 5 Q3: 145 N/A

Test rejected at how many tokens?  
What was the smallest  $p$ -value?  
Quartiles for the distribution of dimension estimates (for those tokens not rejecting manifold hypothesis)

Note: complete lists of all tokens rejecting the hypotheses are in the paper

Do the hypotheses of Theorem 2 apply to each of the four LLMs we tested?

Model	Latent dim $\ell$	Bounding dim. $d$		Context window $w$	Min. output tokens $m$ such that	Singularities persist?	
		Small	Large			Small	Large
GPT2	768	389	14	1024	1038	38	Maybe Yes
Llemma7B	4096	4096	11	4096	8193	23	Maybe Yes
Mistral7B	4096	48	6	4096	97	13	Yes Yes
Pythia6.9B	4096	108	5	4096	217	11	Yes Yes

"Yes" means singularities will persist into LLM output

## Implications

1. Token embeddings are not samples from a low curvature manifold nor from a fiber bundle
2. Irregular tokens may result in instabilities in LLM output  
Small changes in a prompt may result in large changes in the response
3. Longer context windows and fine tuning do not resolve these instabilities (Thm 2)
4. This may explain LLM behavioral features:
  - a. Glitch tokens
  - b. Behavior differences between models, could be useful for model attribution



## References

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Code Paper



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