

## Problem

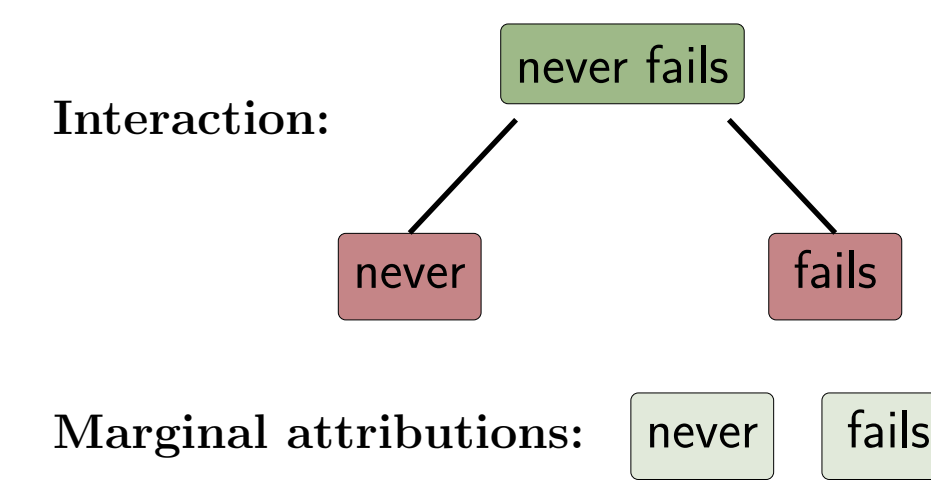
How can we efficiently identify the influential feature interactions in LLMs?

### (a) SENTIMENT ANALYSIS

**CONTEXT**  
... Her acting never fails to impress. She brings depth and authenticity to every role. Her performances consistently draw the ...

**PROMPT**  
Is this a positive or negative review?

**GENERATED RESPONSE**  
Positive.

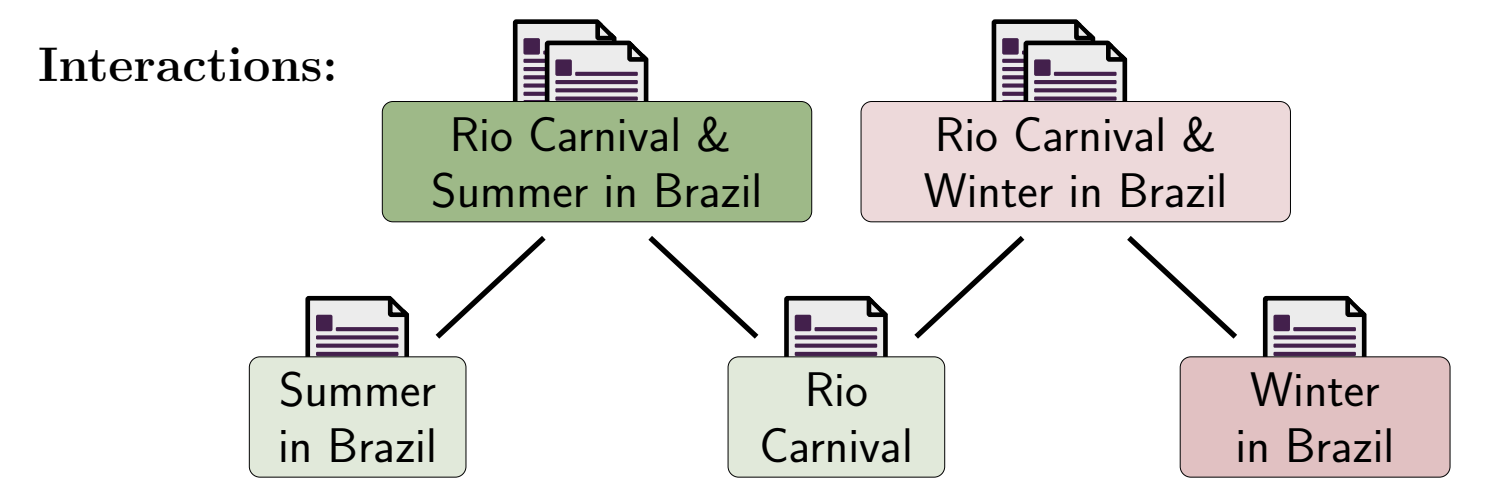


### (b) RETRIEVAL AUGMENTED GENERATION

**CONTEXT**  
... Weather in Tokyo Brazilian Music Rio Carnival Summer in Brazil Winter in Brazil History of Brazil Sport in Rio ...

**PROMPT**  
What is the weather like during Rio Carnival?

**GENERATED RESPONSE**  
Rio Carnival generally takes place during the summer season in Brazil. The weather at this time is typically hot and humid.



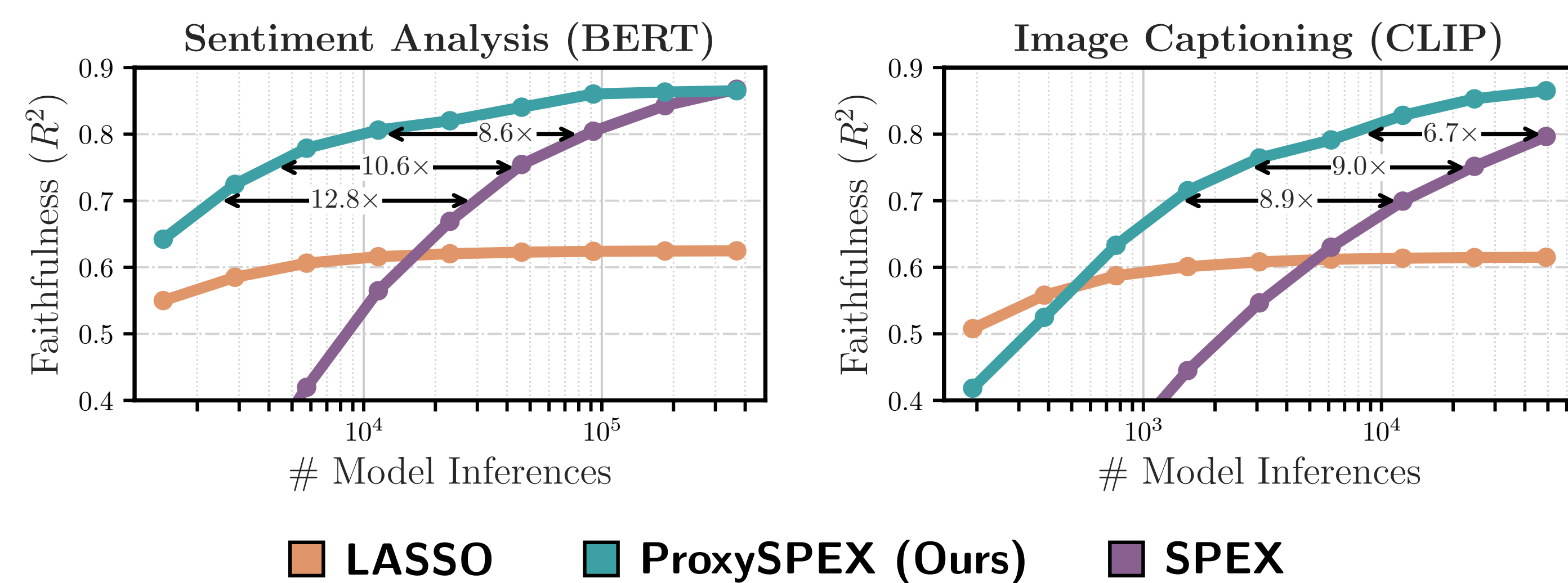
- **Examples:** double negatives in sentiment analysis tasks and multi-document understanding in question answering tasks.
- Marginal attribution approaches like SHAP/LIME scale, but don't capture important interactions.
- A prior approach (SPEX) scales, but still requires tens of thousands of model inferences, which can be prohibitive for complex models such as LLMs.

## Faithfulness at Scale

- For input  $\mathbf{x} = \text{"Her acting fails to impress"}$ , let  $f(\mathbf{x}_S)$  be the output of the LLM under *masking pattern*  $S$ .
- If  $S = \{1, 2, 4, 5, 6\}$ , then  $\mathbf{x}_S$  is "Her acting [MASK] fails to impress". This masking pattern changes the sentiment score from positive to negative.
- We aim to learn an interpretable approximate function  $\hat{f}$  that is faithful to the original function  $f$ , measured in terms of  $R^2$ :

$$R^2 = 1 - \frac{\|\hat{f} - f\|^2}{\|f - \bar{f}\|^2}, \quad \text{where } \|f\|^2 = \sum_{S \subseteq [n]} f(S)^2, \quad \bar{f} = \frac{1}{2^n} \sum_{S \subseteq [n]} f(S).$$

**Result:** ProxySPEX requires  $\sim 10\times$  fewer inferences to achieve equally faithful explanations as SPEX.



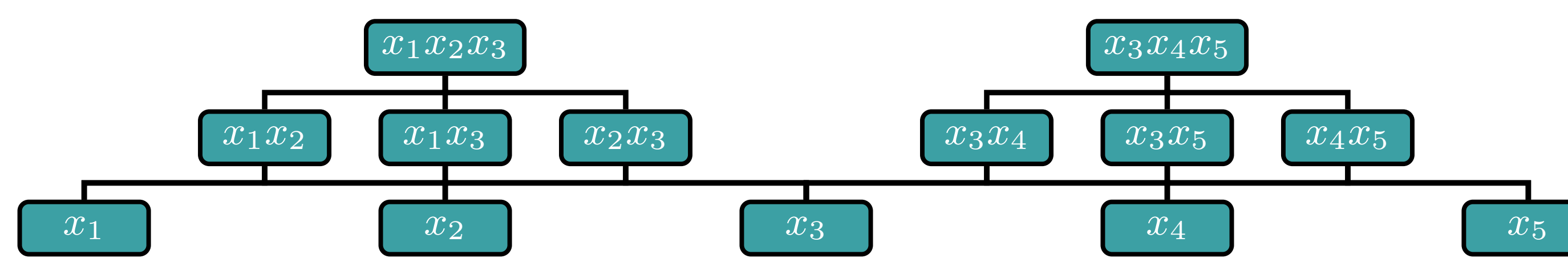
## Fourier Sparsity and Spectral Hierarchies

- Every function  $f(\mathbf{x}_S)$  has a unique decomposition under the Fourier transform, expressed as:

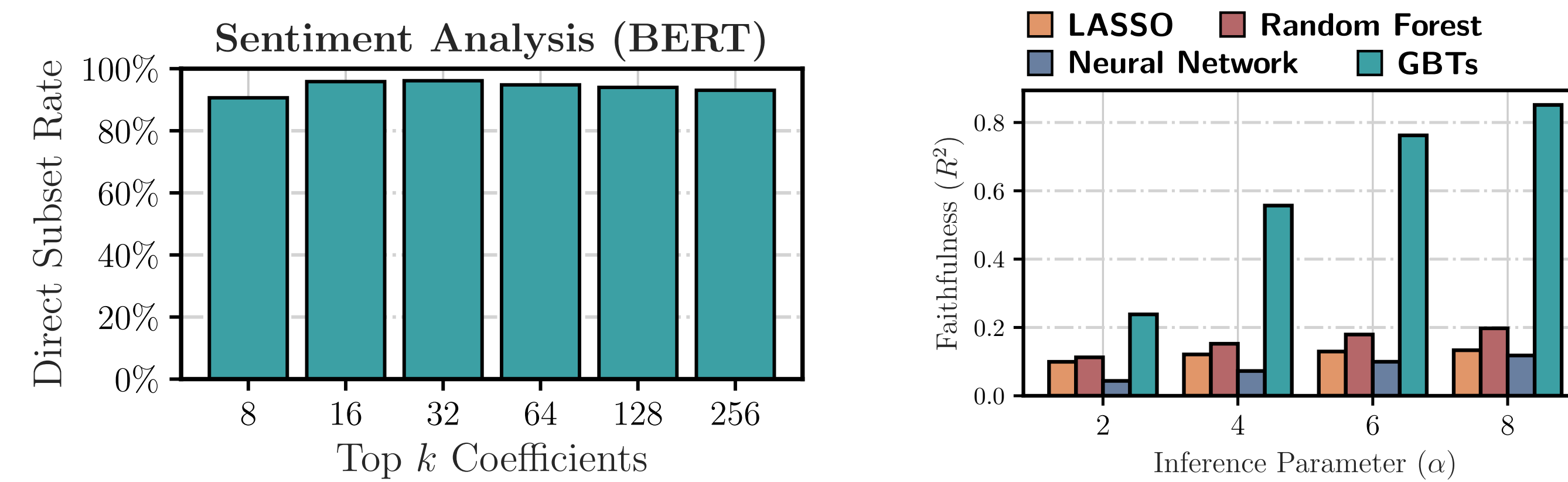
$$F(\mathbf{x}_T) = \frac{1}{2^n} \sum_{S \subseteq [n]} (-1)^{|S \cap T|} f(\mathbf{x}_S), \quad f(\mathbf{x}_S) = \sum_{T \subseteq [n]} (-1)^{|S \cap T|} F(\mathbf{x}_T).$$

- It has been observed that  $F(\mathbf{x}_T) \approx 0$  for most  $T$  (sparsity), and most large  $F(\mathbf{x}_T)$  are **low degree** such that  $|T| \leq d$  for some small  $d$ .

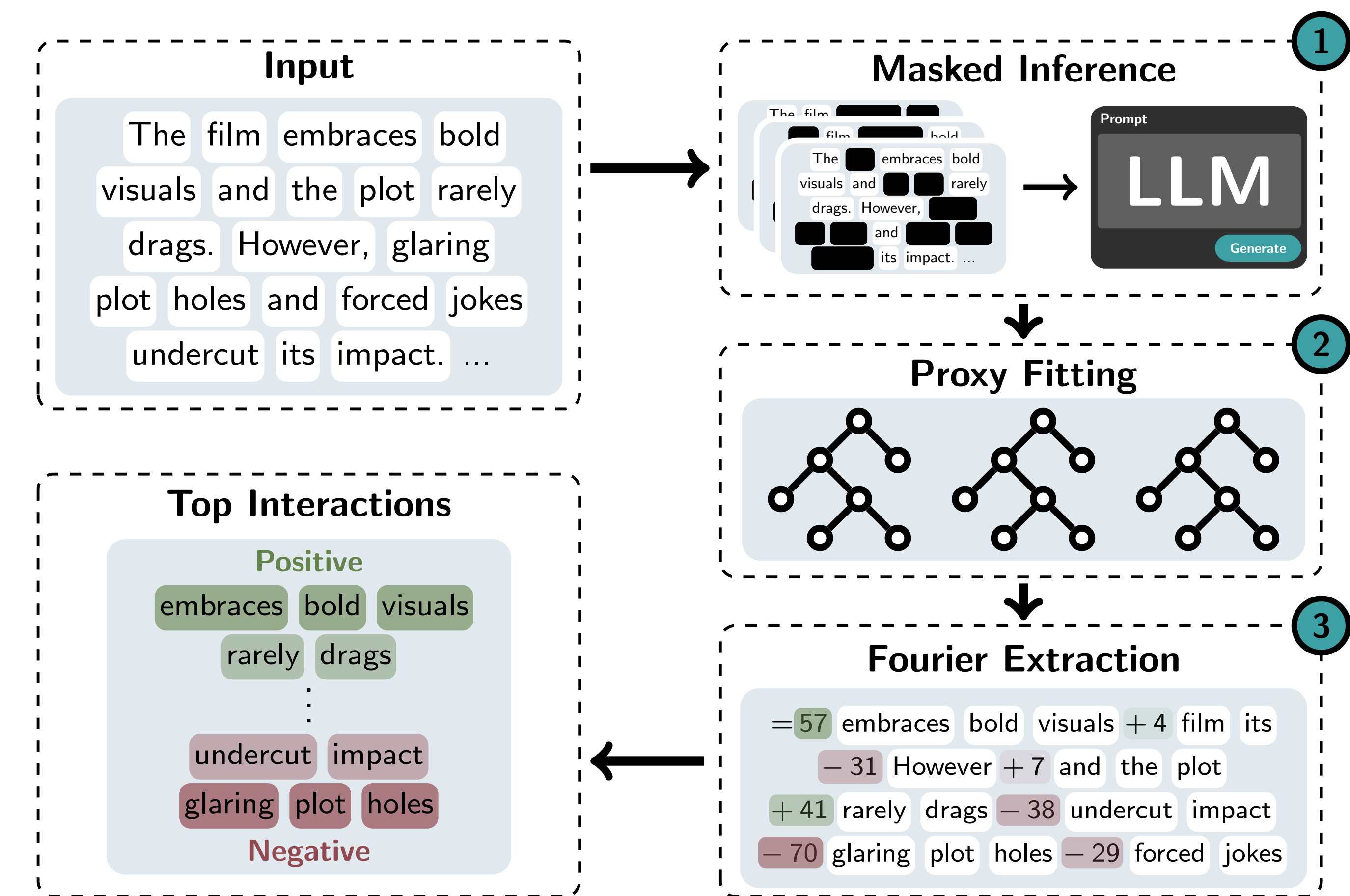
In addition to **sparse** and **low-degree**, influential interactions are **hierarchical**: higher-order interactions are accompanied by their lower-order subsets.



(Left) Direct subset rate measures the rate at which a top- $k$  interaction has a lower-order subset also contained in the top- $k$ . (Right) Gradient Boosted Trees efficiently recover sparse, hierarchical interactions.

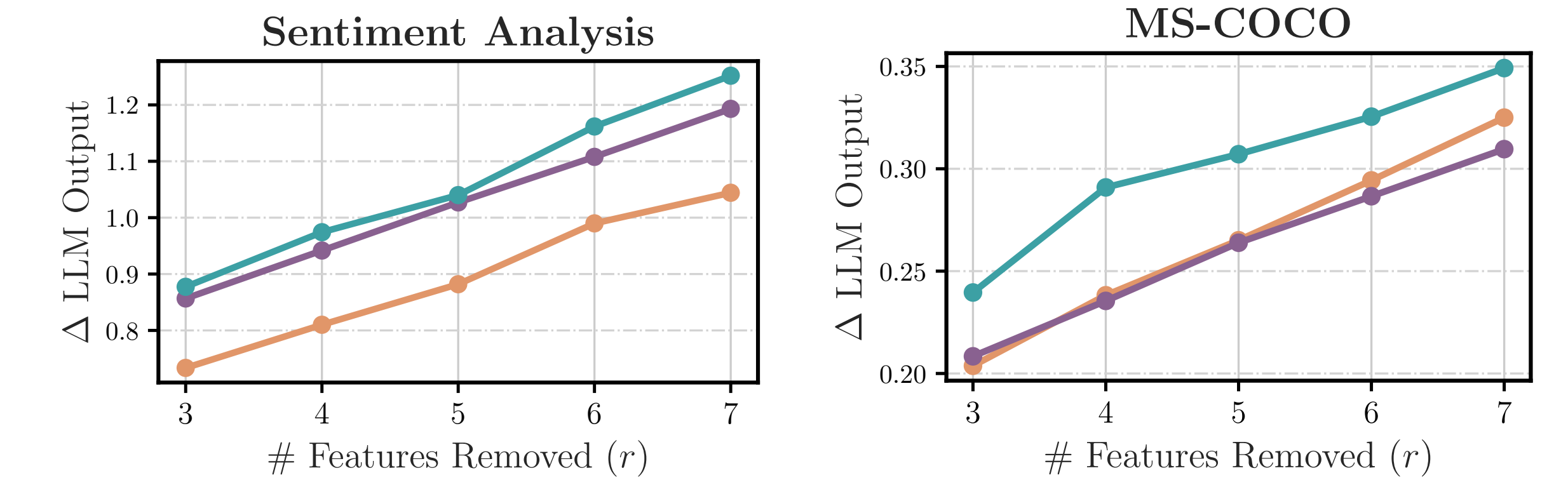


## ProxySPEX Algorithm



- (1) ProxySPEX masks subsets of words and queries the LLM using this masked input.
- (2) It then fits Gradient Boosted Trees as a proxy model to learn the LLM's hierarchical interactions.
- (3) A sparse representation is extracted from the fitted GBTs, capturing influential interactions.

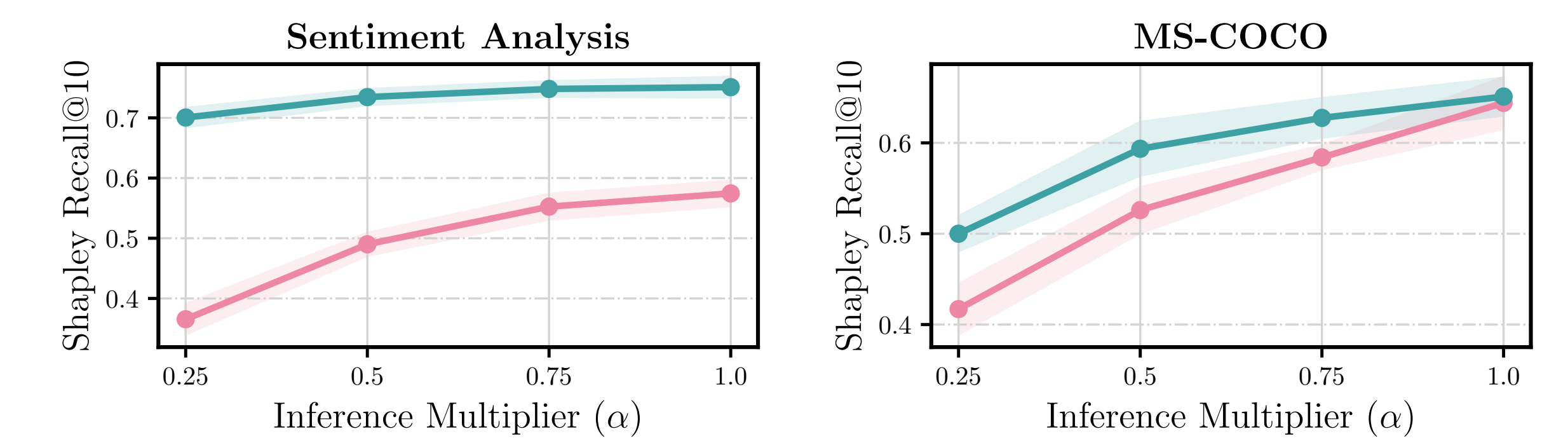
## Feature Removal



Legend: LASSO (orange), ProxySPEX (Ours) (teal), SPEX (purple)

By accounting for interactions, ProxySPEX identifies more influential features across datasets than the LASSO and SPEX.

## Sample-Efficient Shapley Estimation

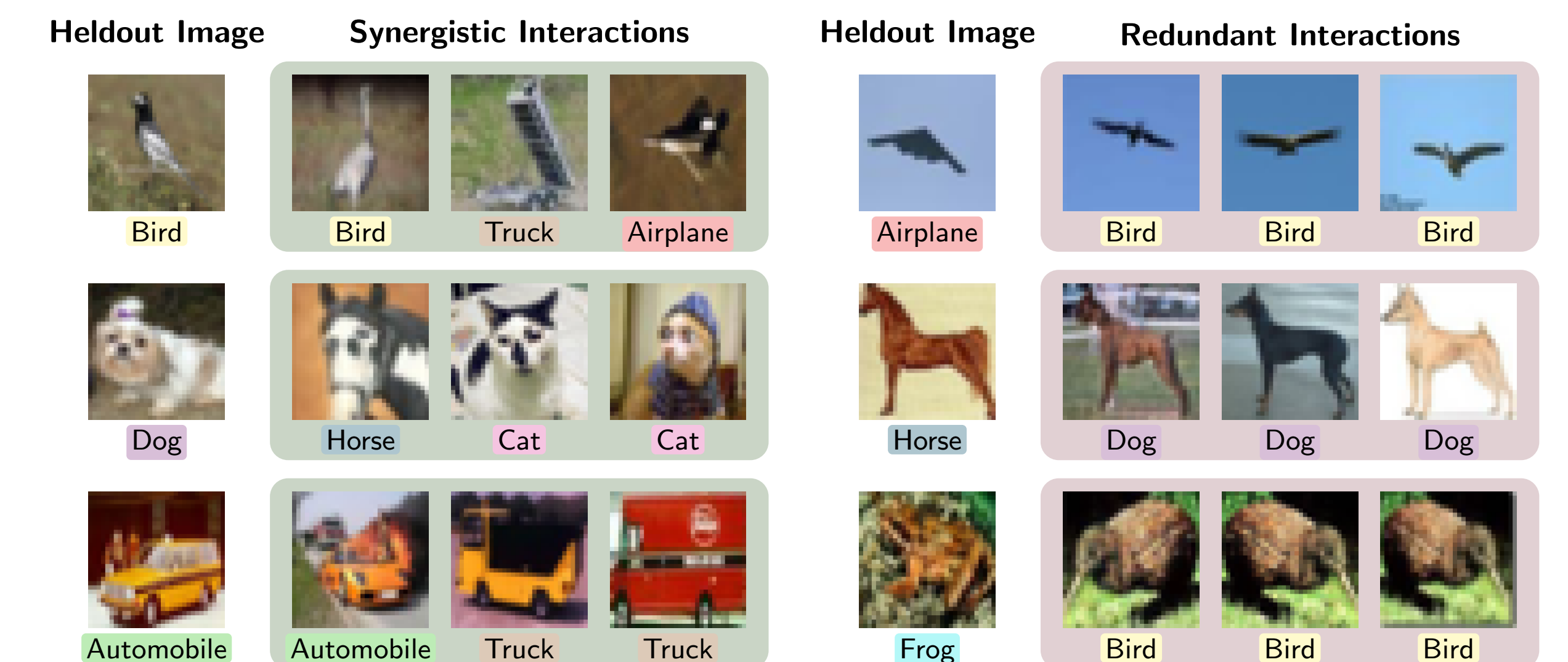


Legend: KernelSHAP (pink), ProxySPEX (Ours) (teal)

For multipliers  $\alpha \in \{0.25, 0.5, 0.75, 1.0\}$ , recall of the top ten Shapley values after  $\alpha \cdot n \log_2(n)$  inferences. For small  $\alpha$ , ProxySPEX is **superior at recovering the most significant features**, while KernelSHAP outperforms as  $\alpha$  increases.

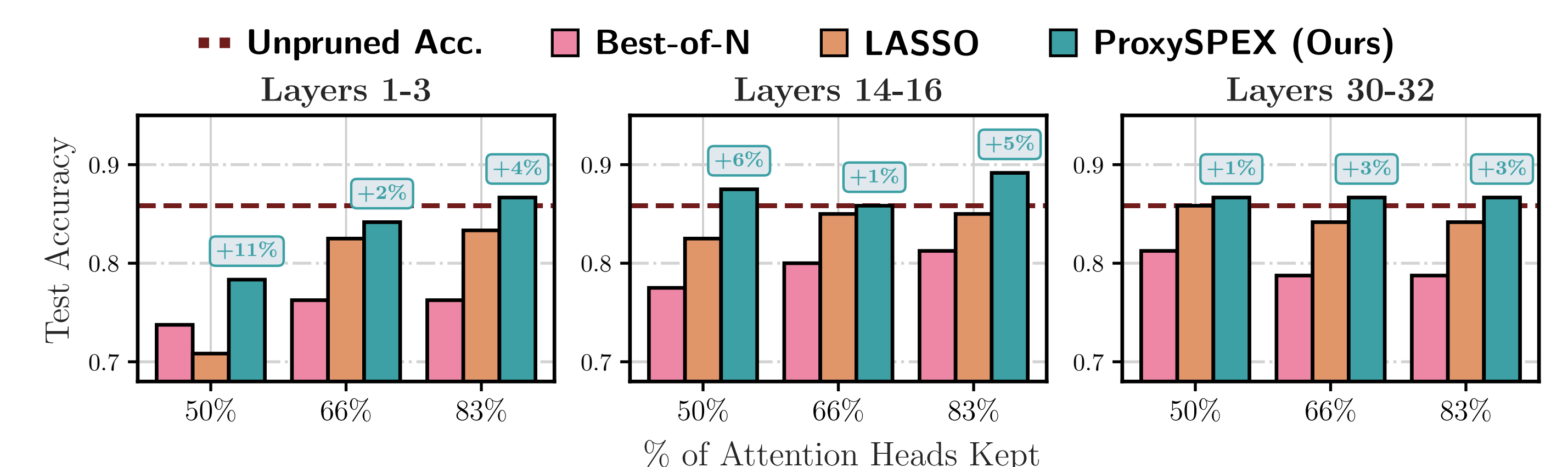
## Data Interaction Attribution

Data attribution measures how each training sample influences the prediction of a particular test point. We extend this framework to capture interactions.



**Synergistic interactions:** data that together are more valuable together than the sum of their parts. **Redundant interactions:** Combined influence is less than the sum of the parts.

## Attention Head Interaction Attribution



Attention head pruning for **Llama-3.1-8B-Instruct** for MMLU (high-school-us-history) across different layers. Unpruned accuracy shown by dashed line.