

Improving LLM Attributions with Randomized Path-Integration

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Abstract

We present Randomized Path-Integration (RPI) - a path-integration method for explaining language models via randomization of the integration path over the attention information in the model. RPI employs integration on internal attention scores and their gradients along a randomized path, which is dynamically established between a baseline representation and the attention scores of the model. The inherent randomness in the integration path originates from modeling the baseline representation as a randomly drawn tensor from a Gaussian diffusion process. As a consequence, RPI generates diverse baselines, yielding a set of candidate attribution maps. This set facilitates the selection of the most effective attribution map based on the specific metric at hand. We present an extensive evaluation, encompassing 11 explanation methods and 5 language models, including the Llama2 and Mistral models. Our results demonstrate that RPI outperforms latest state-of-the-art methods across 4 datasets and 5 evaluation metrics. Our code is available at: <https://github.com/rpicnf/rpi>

1 Introduction

Recent advancements in AI research have impacted numerous application domains, fueling innovation and progress in user modeling and personalization (Barkan and Koenigstein, 2016; He et al., 2017; Ben-Elazar et al., 2017; Wang et al., 2019; He et al., 2020; Barkan et al., 2019a, 2020a,b,d, 2021d, 2023f; Katz et al., 2022), natural language processing (NLP) (Mikolov et al., 2013; Vaswani et al., 2017; Devlin et al., 2018; Brown et al., 2020; Barkan, 2017; Barkan et al., 2020f,e, 2021b; Ginzburg et al., 2021; Malkiel et al., 2020, 2022b), computer vision (He et al., 2016; Dosovitskiy et al., 2020; Liu et al., 2022; Carion et al., 2020; Assran

et al., 2023; Barkan et al., 2023e), and sound synthesis (Engel et al., 2020; Kong et al., 2020; Barkan and Tsiris, 2019; Barkan et al., 2019b, 2023g).

Within the field of NLP, the advent of Transformers (Vaswani et al., 2017; Devlin et al., 2018; Radford et al., 2019) have ushered in a new era of complex language model (LM) architectures (Liu et al., 2019; Raffel et al., 2019; Brown et al., 2020; Touvron et al., 2023). These models, with their expanding size and complexity, have become integral components across diverse applications.

This surge in model capacity and complexity has intensified the need for a profound understanding of the decision-making processes intrinsic to LMs. However, the inherent complexity often shrouds the transparency of these models' predictions, prompting the development of explainability methods to unveil the contributing factors influencing their outputs. Consequently, a multitude of explanation methods has been devised (Ribeiro et al., 2016; Sundararajan et al., 2017; Lundberg and Lee, 2017; Abnar and Zuidema, 2020; Modarressi et al., 2023).

Simultaneously, with the evolution of explanation methods, there has been a proliferation of various explanation metrics designed for the quantitative assessment of explainability methods (Samek et al., 2017; DeYoung et al., 2020). However, achieving consensus within the literature on the ultimate explanation metric remains elusive, as each metric offers unique insights into different facets of explanation quality.

Acknowledging the diversity in explanation metrics, we introduce Randomized Path-Integration (RPI), a method designed to elucidate predictions made by LMs through the integration of internal attention scores and their gradients along a random path. The introduction of randomness into the integration path stems from the representation of the baseline as a random tensor drawn from a

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specified baseline distribution. As a result, RPI produces a variety of baselines from this distribution, forming a pool of candidate attribution maps. The versatility afforded by multiple baselines facilitates the selection of the most effective attribution map, contingent upon the evaluation metric under consideration.

Through extensive evaluation spanning a variety of explanations methods, LMs, and datasets, RPI exhibits superior performance compared to current state-of-the-art methods across multiple explanation metrics.

2 Related Work

Explainable AI includes a wide array of methods, all aimed at improving the understanding of decisions made by deep learning models across multiple application domains (Fong et al., 2019; Simonyan et al., 2013; Fong and Vedaldi, 2017; Selvaraju et al., 2017; Zhou et al., 2018; Barkan et al., 2020c, 2021c,a, 2023d,c,a,b; Gaiger et al., 2023; Barkan et al., 2024; Malkiel et al., 2022a; Chefer et al., 2021a,b; Sanyal et al., 2022).

Perturbation-based techniques such as LIME (Ribeiro et al., 2016) and SHAP (Lundberg and Lee, 2017) introduce perturbations to individual inputs or neurons and observe their consequential effects on subsequent neurons in the network.

Relevance-Decomposition methods look at the network’s representation as vectors, each exerting distinct influences on the model’s predictions. GlobEnc (Modarressi et al., 2022) and ALTI (Ferrando et al., 2022) incorporate local-level decomposition, aggregating resulting vector norms using rollout (Abnar and Zuidema, 2020) to construct global-level explanations. Recently, DecompX (Modarressi et al., 2023) was introduced, providing state-of-the-art results by constructing decomposed token representations and sequentially propagating them through the model without inter-layer mixing.

Gradient-based methods rely on the gradients of the model’s prediction score concerning the input tokens. Basic gradient methods, such as Vanilla Gradients (Simonyan et al., 2013) and GradientXInput (Shrikumar et al., 2016), operate on the principle of gradient computation. Integrated Gradients (IG) (Sundararajan et al., 2017) is a path-

integration method, computing gradients on interpolated points along a straight line between the data and an uninformative baseline. Additional approaches such as DeepLift (Shrikumar et al., 2017) and GradientShap (Lundberg and Lee, 2017) can be viewed as approximations of IG. Other path-integration methods, such as Discretized Integrated Gradient (DIG) (Sanyal and Ren, 2021), treat the integration path differently. DIG replaces the continuous straight path with a discretized one, where interpolated points are words. Another innovative path-integration approach comes in the form of Sequential Integrated Gradients (SIG) (Enguehard, 2023). SIG addresses concerns about altered sentence meaning by computing the importance of each word while keeping other words fixed and creating interpolations between the baseline and the word of interest. Notably, SIG has demonstrated superior performance when compared to several existing methods, including DIG, IG, and GradientShap.

RPI complements this line of path-integration methods by modeling the baseline representation as a random tensor sampled from a Gaussian diffusion process (Sohl-Dickstein et al., 2015), and integrating the attention scores and their gradients along a randomized path between a randomly drawn baseline and the attention scores to form an attribution map. By baseline resampling from the baseline distribution, RPI establishes a pool of candidate attribution maps that facilitates the selection of the most effective attribution map based on the metric under consideration. Our evaluation indicates that this unique feature of RPI leads to state-of-the-art results and can be further incorporated to existing path-integration to enhance their performance.

3 Randomized Path-Integration

Let \mathcal{V} denote the vocabulary, and let $u = (u_i)_{i=1}^k$ represent a sequence of k tokens constituting the input text, where each $u_i \in \mathcal{V}$. We further define $\mathbf{x}_u = [\mathbf{x}_{u_1}, \dots, \mathbf{x}_{u_k}]$ as a 2D tensor in $\mathbb{R}^{d \times k}$ accommodating k embeddings, with each $\mathbf{x}_{u_i} \in \mathbb{R}^d$ representing the token u_i .

In the context of this work, our emphasis lies in the domain of classification tasks. Hence, we introduce a model denoted as F , designed to take an input \mathbf{x}_u and yield an output $F(\mathbf{x}_u) \in [0, 1]^c$. Here, $F_i(\mathbf{x}_u)$ denotes the probability assigned to class i ,

and c signifies the total number of available classes. The model F can assume the form of a LM utilizing a classification head, producing probabilities for each class within the specific task. This process involves either finetuning the LM or utilizing it as a foundational component for the transfer learning of a specific task.

Recent LM architectures, often referred to as large language models (LLMs), are predominantly decoder-based, tasked with completing sequences of tokens in the output (Brown et al., 2020). Although these LLMs can be finetuned using classification heads, a more prevalent approach is classification via completion (Raffel et al., 2019). In this method, the LLM is prompted with the specific task, either in a few-shot or zero-shot scenario, and instructed to generate a token that signifies the correct class. For instance, in sentiment analysis, if the relevant classes are communicated to the LLM (via prompt) as 'positive' and 'negative', logit scores for the tokens 'positive' and 'negative' are computed, and softmax is applied to obtain the probabilities associated with each class. It is noteworthy that this approach can be implemented either before or after finetuning the LLM on the relevant dataset in a completion manner.

In this work, we conduct experiments in various settings, including finetuning with classification heads on top of the LLM as well as classification via completion (decoder-based models).

3.1 Integrated Gradients

IG (Sundararajan et al., 2017) enables the creation of an attribution map by defining a linear path between a baseline representation $\mathbf{b} \in \mathbb{R}^{d \times k}$ and \mathbf{x}_u via the parameterization:

$$\mathbf{v}_u = \mathbf{b} + a(\mathbf{x}_u - \mathbf{b}) \text{ with } a \in [0, 1], \quad (1)$$

and accumulating the gradients along this path as follows:

$$\begin{aligned} \mathbf{m}_{IG} &= \int_0^1 \frac{\partial F_y}{\partial \mathbf{v}_u} \circ \frac{\partial \mathbf{v}_u}{\partial a} da \\ &\approx \frac{\mathbf{x}_u - \mathbf{b}}{n} \circ \sum_{j=1}^n \frac{\partial F_y}{\partial \mathbf{v}_u}, \end{aligned} \quad (2)$$

where \circ denotes the Hadamard product, y denotes the class receiving the highest score in the prediction, and the approximation in the last transition is

obtained by setting $a = \frac{j}{n}$ in Eq. 1. The resulting attribution map \mathbf{m}_{IG} can be manipulated in various ways to form attribution scores for each individual element in \mathbf{x}_u .

3.2 The RPI method

RPI facilitates two distinctive features that set it apart from IG. Firstly, RPI integrates on the internal attention scores (rather than the token representation themselves), computed in the intermediate layers of F , and their gradients. This design allows for the aggregation of information from various attention heads and model layers w.r.t. each individual token in the input. Secondly, RPI models the baseline representation¹ \mathbf{b} as a random tensor drawn from a distribution \mathcal{B} . This approach facilitates the sampling of multiple baselines, resulting in various integration paths, each leading to a distinct attribution map. Subsequently, one can select the attribution map associated with the integration path that yields the best results on the specific explanation metric under consideration. In what follows, we describe RPI in detail.

Let $\mathbf{a}_u^l \in \mathbb{R}^{h \times k \times k}$ denote the attention scores tensor accommodating the h attention matrices produced by the l -th layer in the model F (when applied to a specific input \mathbf{x}_u). With a budget of trials R , the RPI process unfolds as follows: First, we sample R baselines $B^l = \{\mathbf{b}^{lr}\}_{r=1}^R$ from the baseline distribution \mathcal{B} , where $\mathbf{b}^{lr} \in \mathbb{R}^{h \times k \times k}$. Accordingly, we redefine the interpolant for the attention tensor as:

$$\mathbf{v}_u^{lr} = \mathbf{b}^{lr} + a(\mathbf{a}_u^l - \mathbf{b}^{lr}) \text{ with } a \in [0, 1]. \quad (3)$$

Using B , we compute corresponding set of attribution maps $M^l = \{\mathbf{m}^{lr}\}_{r=1}^R$, where

$$\mathbf{m}^{lr} = \phi \left(\frac{\mathbf{a}_u^l - \mathbf{b}^{lr}}{n} \circ \sum_{j=1}^n \frac{\partial F_y}{\partial \mathbf{v}^{lr}} \circ \mathbf{v}^{lr} \right), \quad (4)$$

and ϕ is a function that takes the resulting tensor from the integration process, performs mean reduction on its first dimension (the attention heads dimension), and extracts a specific row from the resulting 2D matrix, producing the d -dimensional attribution map \mathbf{m}^{lr} . In encoder-based models, the

¹Note that now the baseline representation \mathbf{b} should match the dimensions of the attention tensor, which differ from dimensions of the input tensor dimensions.

extracted row is typically the one corresponding to the attention scores of the first token (e.g., in BERT, it is associated with the CLS). In decoder-based models, the extracted row is the last one corresponding to the last token used to generate the next token predicted by the model as part of the completion task².

We further note that the integrand in Eq.4 involves the Hadamard product of the interpolated attention tensor with its gradient. This is another difference from IG (Eq.2) that integrates the gradients only. We found that the multiplication by the interpolated attention tensor further improves the results, as it allows the amplification of elements in which both the gradient and the interpolated attention score are high. This design choice is further supported by the findings from (Selvaraju et al., 2017).

Finally, in the resulting attribution map $\mathbf{m}^{lr} \in \mathbb{R}^d$ (Eq. 4), the i -th entry \mathbf{m}_i^{lr} represents the attribution score assigned to the token u_i (which is the i -th token in the input u).

Next, we describe the attribution map selection process. Let J be a set containing the indexes of layers in F participating the RPI process, and define the unified set of the resulting attribution maps by $M^J = \cup_{l \in J} M^l$. Consequently, the RPI attribution map is determined by:

$$\mathbf{m}_{\text{RPI}} = \operatorname{argmax}_{\mathbf{m} \in M^J} \psi(\mathbf{m}), \quad (5)$$

where ψ represents the metric under consideration³, and $\psi(\mathbf{m})$ denotes the metric score on the attribution map \mathbf{m} . Ultimately, for simplicity, in this work, we opt for applying RPI with $J = \{L\}$, denotes the index of the last layer in F . As demonstrated in Sec. 4.2, this setup consistently produces state-of-the-art results. This setup further aligns with established explanation methodologies (Selvaraju et al., 2017; Caron et al., 2021) that predominantly utilize the final layer of the model for explanation generation. However, it is essential to note that RPI offers the flexibility to utilize all model layers and their combinations (Eq. 5). Therefore, in the

²Recall that in this work, decoder-based models are customized for a classification task by expecting them to predict the correct class with the first predicted token in the completion.

³For a metric that favors lower scores, the operator in Eq. 5 should be changed to argmin .

Appendix (Section A.1), we conduct an exhaustive ablation study, exploring the application of RPI across various layers and their aggregations.

3.2.1 The baseline distribution

In their study (Sturmfels et al., 2020), the authors investigated various baseline representations, without establishing a clear preference for any specific method. Consequently, a reasonable approach would be to define \mathcal{B} as a mixture of distributions accommodating diverse baseline representations, each with its associated weight. In this work, we propose a more simple approach where the baseline is drawn from a Gaussian diffusion process (Sohl-Dickstein et al., 2015). Specifically, we define the baseline distribution at timestamp t as $\mathcal{B}_t = \mathcal{N}(\sqrt{\bar{\alpha}_t} \mathbf{a}_u^l, (1 - \bar{\alpha}_t) \mathbf{I})$, where $\bar{\alpha}_t = \prod_{j=1}^t \alpha_j$, $\alpha_t = 1 - \beta_t$, and $\{\beta_t\}_{t=1}^T$ are parameters defining the variance schedule over T timesteps. Subsequently, each baseline of the R baselines in \mathcal{B}^l is sampled by uniformly selecting timestamp t from $\{1, \dots, T\}$ and then drawing a baseline \mathbf{b}^{lr} from \mathcal{B}_t .

The rationale for employing the Gaussian diffusion process to model the baseline as a random tensor is to establish a baseline distribution capable of accommodating diverse levels of noise, contingent upon the timestamp t . Specifically, this approach enables the introduction of small Gaussian noise for smaller values of t , gradually transitioning to higher levels of noise that ultimately converge to the standard normal noise as t increases.

Complexity The computational complexity of IG grows linearly with n (number of interpolations), while RPI introduces an additional factor, the number of sampled baselines R , as each baseline entails a different integration path. Fortunately, both IG and RPI are embarrassingly parallel. Therefore, given a GPU capable of accommodating a batch size of nR examples, IG and RPI are anticipated to exhibit comparable runtime performance in practical scenarios. Moreover, our empirical evaluation indicates that, even with a relatively small R , RPI consistently outperforms the latest state-of-the-art explanation methods across a variety of metrics, models, and datasets. Lastly, it is crucial to recognize that explanations serve primarily for debugging and auditing purposes, rather than real-time decision-making. In these contexts, prioritizing the generation of a higher-quality explanation over

speed is often considered advantageous.

4 Experimental Setup and Results

All experiments were conducted on a high-performance NVIDIA DGX server, equipped with 8 A100 GPUs, utilizing the PyTorch platform.

4.1 Experimental setup

Datasets and Models In our comprehensive evaluation, we assess various explanation methods across four distinct datasets, aiming to provide a thorough understanding of their efficacy in diverse scenarios characterized by different classification tasks and text lengths. **SST2** (Socher et al., 2013): Binary sentiment classification focusing on short texts. **Rotten Tomatoes (RTN)** (Pang and Lee, 2005): Binary sentiment classification in medium-sized texts. **Emotion Recognition (EMR)** (Saravia et al., 2018): Emotion classification with six classes (Sadness, Joy, Love, Anger, Fear, and Surprise) predominantly in short texts. **AG News (AGN)** (Zhang et al., 2015): Topic classification with four classes (World, Sports, Business, Sci/Tech) across texts of varying lengths.

Our evaluation involves five distinct model architectures: BERT-Base (Devlin et al., 2018), BERT-Base (Devlin et al., 2018), DistilBERT-Base (Sanh et al., 2019), Llama2 7B (Touvron et al., 2023) and Mistral 7B (Albert Q. Jiang, 2023). For the first three models, we utilize their finetuned versions tailored to each dataset. On the other hand, Llama2 and Mistral were evaluated in few-shot prompting mode without fine-tuning for the RTN and SST2 tasks, which aligns with their typical application in large language models (LLMs), as detailed in Sec. 3. For the AGN and EMR tasks, we finetuned the models using LoRA due to their limited performance in the few-shot prompting scenario. The prompts utilized in this research are presented in the Appendix. The processing of datasets, as well as the retrieval of both pretrained and finetuned versions of models for each dataset, was conducted using the HuggingFace library (Wolf et al., 2019). Our data processing approach closely follows the methodology outlined in (Enguehard, 2023). The complete code for data processing, along with links to access all models, is available in our GitHub repository, ensuring transparency and reproducibility of our research.

Evaluation metrics For quantitative assessment of the explanation methods, we followed the evaluation protocol from recent works (Enguehard, 2023; Ferrando et al., 2022) and report results for the following set of metrics: Log-Odds (**LO**) (Shrikumar et al., 2017), Sufficiency (**Suff**), Comprehensiveness (**Comp**) and Area Over the Perturbation Curve (AOPC) for Sufficiency (**A-S**) and Comprehensiveness (**A-C**) (DeYoung et al., 2020). For Suff, LO and A-S the lower the better, while for Comp and A-C the higher the better. Unless specified otherwise, we use the same metric settings as detailed in the referenced papers. A detailed description of the metrics appears in the Appendix (Sec. A.3).

Explanation methods Our evaluation encompasses 9 explanation methods, representing various approaches in the landscape of model explainability. These methods include: GradientXInput (**GXI**) (Shrikumar et al., 2016), GradientShap (**SHAP**) (Lundberg and Lee, 2017), **LIME** (Ribeiro et al., 2016), DeepLift (**LIFT**) (Shrikumar et al., 2017), Integrated Gradients (**IG**) (Sundararajan et al., 2017), Sequential Integrated Gradients (**SIG**) (Enguehard, 2023), GlobEnc (**GLOB**) (Modarressi et al., 2022), **ALTI** (Ferrando et al., 2022), and Decompx (**DCMP**) (Modarressi et al., 2023). The evaluation adhered to the codebase and hyperparameter search settings provided by the original works for each respective method.

Furthermore, we introduce an explanation method based on the LLM Instruct version (**LLM**). In this approach, we prompt the finetuned, open-source versions of Llama-Instruct and Mistral-Instruct with the task and input, instructing the models to explain the prediction by ranking the importance of each token in the input example. Detailed prompts can be found in our GitHub repository for transparency.

Finally, our RPI method was executed with $R = 24$ and $n = 30$. It is worth noting that the results were observed to be robust as long as $n > 30$. Additionally, the computation of attribution maps \mathbf{m}^{lr} (Eq. 4) utilizes the first row of the attention matrices in the case of BERT, DistilBERT and RoBERTa, and the last row of the attention matrices in Llama2 and Mistral. For the exact implementation details, the reader is referred to our

| Metric | Prediction | Attribution |
|--------|------------|---|
| Suff | Negative | a hideous , <u>confusing</u> spectacle , one that may well put the nail in the coffin of any future rice adaptations. |
| | Positive | a <u>well-made</u> and often lovely depiction of the mysteries of friendship |
| Comp | Negative | a <u>hideous</u> , confusing spectacle , one that may well put the nail in the coffin of any future rice adaptations. |
| | Positive | a well-made and often <u>lovely</u> depiction of the mysteries of friendship |

Table 1: Examples of RPI attributions on several sentences of the SST2 dataset (using the BERT model). The underlined bold words represent the most important tokens in the sentence, while bold words are based on the most important tokens in the sentence, according to the RPI attribution method. The first two and last two rows correspond to the RPI attribution maps that produced the best results for the Suff and Comp metrics, respectively.

GitHub repository.

4.2 Results

We commence with an illustrative example demonstrating that different metrics favor different attributions. Table 1 presents two examples from the SST2 dataset. The first two rows and last two rows visualizes the RPI attribution maps that yielded the best results for the Suff and Comp metrics, respectively, using BERT. In each example, we boldface the top 3 attributed words (according to the generated attribution map), with the word assigned the highest attribution score further underlined. As observed, the best attribution map for each metric differs for the same example. Table 1 illustrates the rationale behind the RPI mechanism, allowing the selection of the most suitable attribution map for each metric. Table 2 presents results for all combinations of encoder-based model, explanation method, dataset, and metric. The findings in Tab 2 consistently highlight the superior performance of RPI across all scenarios, with DCMP and SIG alternating for the second place.

Table 3 illustrates the effectiveness of RPI compared to runner-ups SIG and DCMP from Table 2 on the SST2 dataset using BERT and RoBERTa. The top three attributed words are extracted for each example based on the explanation method. It is evident that RPI produces attributions that align most closely with the predictions. Additional qualitative examples are provided in the Appendix (Sec. A.2).

Table 4 presents quantitative results for the Llama2 and Mistral models. It is important to note that the ALTI and DCMP methods are not

compatible with these models and are therefore excluded from comparison. Similar trends to Tab. 2 emerge, with RPI consistently outperforming other methods by a significant margin in all cases. The runner-up is typically SIG. We also observe that the LLM-based explanation method consistently underperforms compared to the leading explanation methods. This underperformance can be attributed to frequent hallucinations, where the model outputs a ranked token list which includes tokens that are not present in the original input. Overall, the results in Tabs. 2 and 4 establish RPI as the new state-of-the-art method.

4.3 Ablation study

In what follows, we present an ablation study for different configuration choices in RPI. Unless specified otherwise, we used $R = 24$, $n = 30$ and the baselines are drawn from a Gaussian diffusion process. The study was conducted on the RTN dataset, utilizing a finetuned BERT model. Table 6 compares various ablated versions of RPI and explores the impact of applying the RPI baseline resampling procedure to other path-integration methods (IG and SIG). First, we evaluate RPI-G, where attention gradients are used without multiplication in the attention scores (omitting the multiplication in ∇l_r in Eq.4). Second, we assess RPI-IG and RPI-SIG, which incorporate the RPI baseline resampling procedure into IG and SIG methods, respectively. Here, we replace the fixed <MASK> baseline (Enguehard, 2023) with a random baseline drawn from the Gaussian diffusion process (as described in Sec. 3.2.1), while setting \mathbf{a}_u^l to the <MASK> token.

| | | RoBERTa | | | | | DistilBERT | | | | | BERT | | | | |
|------|--------------|---------------|---------------|--------------|--------------|--------------|---------------|---------------|--------------|--------------|--------------|---------------|---------------|--------------|---------------|--------------|
| | | Suff↓ | LO↓ | Comp↑ | A-S↓ | A-C↑ | Suff↓ | LO↓ | Comp↑ | A-S↓ | A-C↑ | Suff↓ | LO↓ | Comp↑ | A-S↓ | A-C↑ |
| SST2 | RPI | -0.007 | -1.691 | 0.491 | 0.008 | 0.250 | -0.010 | -2.200 | 0.524 | 0.004 | 0.266 | -0.019 | -1.743 | 0.549 | -0.003 | 0.282 |
| | SIG | 0.097 | -1.340 | 0.381 | 0.066 | 0.205 | 0.064 | <u>-1.920</u> | <u>0.453</u> | 0.051 | <u>0.242</u> | 0.083 | -1.133 | 0.378 | 0.063 | 0.208 |
| | ALTI | 0.116 | -1.043 | 0.305 | 0.070 | 0.166 | <u>0.059</u> | -1.407 | <u>0.368</u> | <u>0.047</u> | 0.205 | 0.093 | -0.816 | 0.320 | 0.064 | 0.175 |
| | DCMP | 0.086 | <u>-1.366</u> | <u>0.393</u> | 0.057 | <u>0.216</u> | 0.359 | -0.321 | 0.089 | 0.201 | 0.063 | <u>0.037</u> | <u>-1.450</u> | <u>0.467</u> | <u>0.030</u> | <u>0.253</u> |
| | LIFT | 0.331 | -0.300 | 0.098 | 0.189 | 0.060 | 0.234 | -0.605 | 0.162 | 0.140 | 0.098 | 0.289 | -0.314 | 0.118 | 0.168 | 0.071 |
| | GLOB | 0.227 | -0.489 | 0.166 | 0.136 | 0.100 | 0.357 | -0.262 | 0.073 | 0.199 | 0.060 | 0.233 | -0.388 | 0.153 | 0.140 | 0.104 |
| | SHAP | 0.227 | -0.788 | 0.226 | 0.135 | 0.131 | 0.207 | -1.264 | 0.291 | 0.122 | 0.167 | 0.250 | -0.534 | 0.191 | 0.145 | 0.111 |
| | GXI | 0.359 | -0.245 | 0.077 | 0.200 | 0.049 | 0.305 | -0.415 | 0.111 | 0.179 | 0.066 | 0.237 | -0.401 | 0.153 | 0.140 | 0.094 |
| | IG | 0.116 | -1.249 | 0.360 | 0.073 | 0.200 | 0.100 | -1.823 | 0.415 | 0.065 | 0.229 | 0.110 | -0.936 | 0.334 | 0.075 | 0.187 |
| LIME | <u>0.050</u> | -1.180 | 0.356 | <u>0.035</u> | 0.194 | 0.150 | -1.281 | 0.298 | 0.104 | 0.162 | 0.134 | -0.713 | 0.273 | 0.093 | 0.149 | |
| RTN | RPI | -0.029 | -0.961 | 0.449 | 0.035 | 0.218 | -0.034 | -0.559 | 0.390 | 0.033 | 0.186 | -0.019 | -2.675 | 0.622 | 0.002 | 0.319 |
| | SIG | <u>0.114</u> | <u>-0.752</u> | <u>0.324</u> | 0.088 | 0.178 | <u>0.087</u> | -0.520 | 0.316 | <u>0.065</u> | 0.169 | 0.157 | -1.524 | 0.353 | 0.109 | 0.190 |
| | ALTI | 0.146 | -0.489 | 0.228 | 0.103 | 0.131 | 0.119 | -0.428 | 0.206 | 0.084 | 0.117 | 0.111 | -1.266 | 0.334 | 0.079 | 0.193 |
| | DCMP | 0.072 | -0.695 | 0.314 | <u>0.062</u> | <u>0.181</u> | 0.294 | -0.291 | 0.068 | 0.169 | 0.045 | <u>0.045</u> | <u>-2.058</u> | <u>0.471</u> | <u>0.042</u> | <u>0.263</u> |
| | LIFT | 0.374 | -0.142 | 0.059 | 0.209 | 0.040 | 0.232 | -0.322 | 0.095 | 0.145 | 0.060 | 0.310 | -0.523 | 0.155 | 0.183 | 0.092 |
| | GLOB | 0.229 | -0.277 | 0.139 | 0.138 | 0.088 | 0.309 | -0.273 | 0.046 | 0.174 | 0.035 | 0.269 | -0.589 | 0.179 | 0.170 | 0.112 |
| | SHAP | 0.218 | -0.418 | 0.188 | 0.139 | 0.111 | 0.171 | -0.431 | 0.213 | 0.105 | 0.123 | 0.310 | -0.744 | 0.181 | 0.185 | 0.111 |
| | GXI | 0.384 | -0.096 | 0.051 | 0.215 | 0.034 | 0.290 | -0.283 | 0.060 | 0.172 | 0.037 | 0.265 | -0.652 | 0.173 | 0.163 | 0.102 |
| | IG | 0.121 | -0.700 | 0.316 | 0.092 | 0.177 | 0.095 | <u>-0.523</u> | <u>0.322</u> | 0.068 | <u>0.173</u> | 0.183 | -1.117 | 0.278 | 0.123 | 0.169 |
| LIME | 0.117 | -0.471 | 0.242 | 0.086 | 0.137 | 0.099 | -0.469 | 0.269 | 0.072 | 0.145 | 0.186 | -1.023 | 0.261 | 0.124 | 0.146 | |
| AGN | RPI | -0.015 | -0.814 | 0.197 | 0.026 | 0.117 | -0.008 | -1.480 | 0.266 | 0.007 | 0.150 | -0.006 | -1.357 | 0.231 | 0.009 | 0.146 |
| | SIG | 0.066 | -0.664 | 0.173 | 0.105 | 0.110 | 0.088 | -1.089 | 0.179 | 0.111 | 0.107 | 0.041 | -1.422 | 0.265 | 0.070 | 0.163 |
| | ALTI | 0.058 | -0.724 | 0.171 | 0.080 | <u>0.126</u> | <u>0.048</u> | -1.076 | <u>0.191</u> | <u>0.063</u> | <u>0.143</u> | 0.039 | -1.443 | <u>0.273</u> | 0.059 | 0.192 |
| | DCMP | <u>0.008</u> | -1.762 | 0.388 | 0.023 | 0.243 | 0.300 | -0.216 | 0.043 | 0.232 | 0.037 | <u>0.002</u> | -2.656 | 0.445 | <u>0.027</u> | 0.268 |
| | LIFT | 0.221 | -0.186 | 0.047 | 0.205 | 0.036 | 0.202 | -0.327 | 0.062 | 0.175 | 0.039 | 0.308 | -0.592 | 0.110 | 0.241 | 0.067 |
| | GLOB | 0.110 | -0.356 | 0.086 | 0.120 | 0.065 | 0.167 | -0.285 | 0.054 | 0.205 | 0.047 | 0.074 | -0.824 | 0.161 | 0.087 | 0.126 |
| | SHAP | 0.201 | -0.418 | 0.098 | 0.174 | 0.068 | 0.212 | -0.710 | 0.115 | 0.166 | 0.079 | 0.223 | -0.927 | 0.159 | 0.180 | 0.111 |
| | GXI | 0.347 | -0.079 | 0.014 | 0.268 | 0.013 | 0.233 | -0.229 | 0.042 | 0.208 | 0.028 | 0.085 | -1.143 | 0.222 | 0.101 | 0.141 |
| | IG | 0.088 | -0.543 | 0.144 | 0.090 | 0.100 | 0.085 | <u>-1.179</u> | 0.190 | 0.070 | 0.129 | 0.060 | <u>-1.537</u> | 0.264 | 0.069 | 0.177 |
| LIME | 0.105 | -0.483 | 0.119 | 0.114 | 0.075 | 0.096 | -0.527 | 0.096 | 0.119 | 0.062 | 0.136 | -0.347 | 0.066 | 0.147 | 0.044 | |
| EMR | RPI | 0.163 | -4.449 | 0.668 | 0.133 | 0.350 | 0.007 | -2.400 | 0.683 | 0.017 | 0.359 | -0.003 | -4.151 | 0.764 | 0.010 | 0.408 |
| | SIG | 0.347 | -2.006 | 0.438 | 0.214 | 0.239 | 0.147 | -1.398 | 0.494 | 0.091 | 0.269 | 0.190 | -2.063 | 0.512 | 0.116 | 0.279 |
| | ALTI | <u>0.172</u> | -3.144 | 0.608 | 0.129 | 0.338 | <u>0.051</u> | -1.635 | 0.562 | <u>0.036</u> | 0.307 | <u>0.044</u> | -2.592 | <u>0.631</u> | <u>0.030</u> | <u>0.350</u> |
| | DCMP | <u>0.172</u> | -3.326 | 0.622 | 0.129 | 0.337 | 0.537 | -0.370 | 0.118 | 0.278 | 0.082 | 0.060 | -2.763 | 0.625 | 0.044 | 0.346 |
| | LIFT | 0.514 | -2.020 | 0.332 | 0.282 | 0.183 | 0.362 | -0.891 | 0.287 | 0.198 | 0.157 | 0.380 | -1.422 | 0.311 | 0.207 | 0.174 |
| | GLOB | 0.211 | -3.106 | 0.581 | 0.146 | 0.322 | 0.543 | -0.369 | 0.120 | 0.278 | 0.084 | 0.094 | -2.423 | 0.583 | 0.061 | 0.322 |
| | SHAP | 0.525 | -1.293 | 0.254 | 0.288 | 0.151 | 0.307 | -1.024 | 0.337 | 0.169 | 0.186 | 0.426 | -1.157 | 0.278 | 0.228 | 0.167 |
| | GXI | 0.541 | -1.510 | 0.258 | 0.294 | 0.147 | 0.415 | -0.754 | 0.237 | 0.233 | 0.127 | 0.354 | -1.472 | 0.330 | 0.197 | 0.187 |
| | IG | 0.328 | -1.917 | 0.431 | 0.205 | 0.237 | 0.139 | -1.396 | 0.498 | 0.086 | 0.269 | 0.190 | -2.106 | 0.523 | 0.113 | 0.285 |
| LIME | 0.198 | <u>-3.814</u> | <u>0.647</u> | 0.143 | 0.351 | 0.059 | <u>-1.911</u> | <u>0.593</u> | 0.041 | <u>0.320</u> | 0.104 | <u>-2.897</u> | 0.586 | 0.065 | 0.322 | |

Table 2: Evaluation results for all combinations of encoder-based model, dataset, explanation method, and metric. See the notations in Sec. 4.

The results in Tab. 6 indicate that each component in RPI plays a vital yet complementary role, with the baseline resampling procedure showing potential to enhance other path-integration methods. First, RPI-G outperforms RPI-IG, indicating that integration on attention gradients is preferable to integration on the input (as done in IG). Secondly, RPI outperforms RPI-G, demonstrating the benefit of multiplying attention gradients in the attention scores, validating the specific construction of the attribution map in Eq.4. Third, RPI-SIG and RPI-IG outperform SIG and IG, respectively,

showcasing the effectiveness of incorporating the RPI baseline resampling procedure. However, both RPI-SIG and RPI-IG fall short compared to RPI, emphasizing the effectiveness of our proposed RPI and the complementary contribution of the RPI baseline resampling procedure along with the attention level integration and the attention scores multiplication. Overall, these findings underscore the efficacy of the RPI baseline resampling procedure as a meta-method to improve performance when applied on top of path-integration methods, and the superiority of the specific RPI implementation pro-

| Dataset | Prediction | Model | Method | Attribution |
|---------|------------|---------|--------|---|
| SST2 | Positive | BERT | RPI | a modest pleasure that accomplishes its goals with ease and confidence . |
| | | | SIG | a modest pleasure that accomplishes its goals with ease and confidence . |
| | | | DCMP | a modest pleasure that accomplishes its goals with ease and confidence . |
| SST2 | Negative | BERT | RPI | apallingly absurd ... the chemistry or lack thereof between newton and wahlberg could turn an imax theater into a 9 '' black and white portable tv . |
| | | | SIG | apallingly absurd ... the chemistry or lack thereof between newton and wahlberg could turn an imax theater into a 9 '' black and white portable tv . |
| | | | DCMP | apallingly absurd ... the chemistry or lack thereof between newton and wahlberg could turn an imax theater into a 9 '' black and white portable tv . |
| SST2 | Positive | RoBERTa | RPI | not ' terrible filmmaking ' bad , but more like , ' i once had a nightmare like this , and it 's now coming true ' bad . |
| | | | SIG | not ' terrible filmmaking ' bad , but more like , ' i once had a nightmare like this , and it 's now coming true ' bad . |
| | | | DCMP | not ' terrible filmmaking ' bad , but more like , ' i once had a nightmare like this , and it 's now coming true ' bad . |

Table 3: Examples of attributions on sentences from the SST2 dataset. The bold words represent the top 3 words in the sentence, according to each attribution method.

| | | Llama2 | | | | | Mistral | | | | |
|------|------|--------------|---------------|--------------|--------------|--------------|---------------|---------------|--------------|--------------|--------------|
| | | Suff↓ | LO↓ | Comp↑ | A-S↓ | A-C↑ | Suff↓ | LO↓ | Comp↑ | A-S↓ | A-C↑ |
| SST2 | RPI | 0.137 | -0.104 | 0.069 | 0.083 | 0.041 | 0.205 | -0.299 | 0.208 | 0.139 | 0.105 |
| | SIG | 0.157 | -0.098 | 0.065 | 0.090 | <u>0.041</u> | 0.281 | <u>-0.256</u> | <u>0.176</u> | 0.160 | <u>0.100</u> |
| | LIFT | 0.159 | -0.056 | 0.033 | 0.093 | 0.023 | 0.319 | -0.139 | 0.100 | 0.184 | 0.067 |
| | SHAP | 0.152 | -0.072 | 0.048 | 0.088 | 0.032 | 0.308 | -0.125 | 0.090 | 0.177 | 0.061 |
| | GXI | 0.159 | -0.054 | 0.033 | 0.092 | 0.023 | 0.319 | -0.142 | 0.102 | 0.184 | 0.067 |
| | LLM | 0.119 | <u>-0.101</u> | <u>0.069</u> | 0.069 | 0.042 | <u>0.257</u> | -0.115 | 0.082 | <u>0.151</u> | 0.062 |
| RTN | RPI | <u>0.177</u> | -0.176 | 0.103 | <u>0.112</u> | 0.061 | 0.189 | -0.458 | 0.275 | 0.150 | 0.138 |
| | SIG | 0.219 | -0.146 | 0.088 | 0.126 | 0.054 | <u>0.312</u> | <u>-0.323</u> | <u>0.215</u> | <u>0.184</u> | <u>0.121</u> |
| | LIFT | 0.211 | -0.115 | 0.068 | 0.124 | 0.040 | 0.375 | -0.156 | 0.103 | 0.220 | 0.077 |
| | SHAP | 0.216 | -0.103 | 0.059 | 0.124 | 0.043 | 0.365 | -0.140 | 0.097 | 0.213 | 0.068 |
| | GXI | 0.212 | -0.114 | 0.066 | 0.125 | 0.040 | 0.375 | -0.161 | 0.105 | 0.220 | 0.077 |
| | LLM | 0.172 | <u>-0.152</u> | <u>0.091</u> | 0.104 | <u>0.056</u> | 0.323 | -0.129 | 0.083 | 0.191 | 0.065 |
| AGN | RPI | 0.008 | -1.375 | 0.242 | 0.115 | 0.142 | -0.008 | -2.384 | 0.305 | 0.069 | 0.185 |
| | SIG | 0.386 | -0.367 | <u>0.081</u> | 0.298 | <u>0.054</u> | 0.365 | <u>-0.750</u> | <u>0.123</u> | 0.295 | <u>0.077</u> |
| | LIFT | 0.414 | -0.561 | 0.059 | 0.312 | 0.041 | 0.447 | -0.487 | 0.070 | 0.334 | 0.048 |
| | SHAP | 0.361 | -0.447 | 0.055 | 0.291 | 0.041 | 0.401 | -0.396 | 0.063 | 0.311 | 0.046 |
| | GXI | 0.423 | -0.564 | 0.058 | 0.314 | 0.040 | 0.447 | -0.489 | 0.067 | 0.335 | 0.048 |
| | LLM | <u>0.252</u> | <u>-0.643</u> | 0.047 | <u>0.246</u> | 0.039 | <u>0.359</u> | -0.226 | 0.042 | <u>0.295</u> | 0.040 |
| EMR | RPI | 0.259 | -4.272 | 0.803 | 0.195 | 0.425 | 0.130 | -5.679 | 0.766 | 0.117 | 0.396 |
| | SIG | <u>0.469</u> | <u>-1.879</u> | <u>0.584</u> | <u>0.272</u> | <u>0.302</u> | 0.273 | <u>-2.572</u> | 0.620 | 0.174 | 0.336 |
| | LIFT | 0.661 | -1.563 | 0.456 | 0.370 | 0.252 | 0.629 | -1.697 | 0.367 | 0.344 | 0.204 |
| | SHAP | 0.632 | -1.316 | 0.386 | 0.344 | 0.216 | 0.451 | -2.001 | 0.452 | 0.255 | 0.251 |
| | GXI | 0.663 | -1.566 | 0.457 | 0.369 | 0.252 | 0.629 | -1.683 | 0.367 | 0.344 | 0.205 |
| | LLM | 0.701 | -0.773 | 0.204 | 0.364 | 0.124 | 0.561 | -1.306 | 0.303 | 0.281 | 0.185 |

Table 4: Evaluation results on the Llama2 and Mistral models.

| R | Suff↓ | LO↓ | Comp↑ | A-S↓ | A-C↑ |
|------|---------------|---------------|--------------|--------------|--------------|
| R=1 | 0.254 | -0.885 | 0.239 | 0.154 | 0.135 |
| R=2 | 0.097 | -1.270 | 0.342 | 0.078 | 0.181 |
| R=4 | 0.020 | -1.725 | 0.447 | 0.037 | 0.233 |
| R=8 | -0.008 | -2.232 | 0.534 | 0.017 | 0.277 |
| R=16 | -0.016 | -2.487 | 0.600 | 0.007 | 0.304 |
| R=24 | <u>-0.019</u> | <u>-2.675</u> | <u>0.622</u> | <u>0.002</u> | <u>0.319</u> |
| R=32 | -0.019 | -2.820 | 0.636 | 0.000 | 0.329 |

Table 5: Ablation Study: results for different values of R (the number of sampled baselines in RPI) on RTN using the BERT model.

| | Suff↓ | LO↓ | Comp↑ | A-S↓ | A-C↑ |
|---------|---------------|---------------|--------------|--------------|--------------|
| RPI | -0.019 | <u>-2.675</u> | 0.622 | 0.002 | 0.319 |
| RPI-G | 0.000 | -2.642 | 0.584 | 0.017 | 0.319 |
| RPI-SIG | -0.013 | -2.584 | 0.600 | 0.011 | <u>0.323</u> |
| RPI-IG | <u>-0.017</u> | -2.703 | <u>0.614</u> | <u>0.004</u> | 0.329 |
| IG | 0.183 | -1.117 | 0.278 | 0.123 | 0.169 |
| SIG | 0.157 | -1.524 | 0.353 | 0.109 | 0.190 |

Table 6: This ablation study highlights significant and complementary contributions of the components in the RPI method. These include integrating at the attention level (RPI) vs. input level (RPI-IG), the benefit from applying the RPI baseline resampling procedure for other path-integration methods (RPI-SIG vs. SIG, RPI-IG vs. IG), and from multiplying the attention scores in their gradients vs. using the plain gradients (RPI vs. RPI-G). The results show that each component in the our proposed RPI method plays a vital role, with the baseline resampling procedure showing potential to enhance other path-integration methods as well.

posed in this work. Table 5 investigates the impact of varying the number of sampled baselines for $R \in \{1, 2, 4, 8, 16, 24, 32\}$ on RPI’s performance. We observe a slight improvement when increasing the number of trials from 24 to 32, demonstrating that the settings of $R = 24$ are sufficient for achieving state-of-the-art performance while maintaining acceptable runtime. It is noteworthy that although the number of interpolation steps n is also a configurable parameter, increasing it beyond $n = 30$ did not result in a significant improvement.

Lastly, recall that in the general case, RPI supports the inclusion of attribution maps from all layers in the model (Eq. 5). Therefore, in Appendix A.1, we provide a thorough ablation study assessing the performance of RPI when applied to individual layers and when aggregating attribution

maps from multiple layers. Our findings show that performance tends to improve with deeper layers, and top-down layer aggregation performs the best.

5 Conclusion

This work responds to the diversity inherent in explanation metrics, recognizing that different metrics may promote different attribution maps. RPI effectively addresses this challenge by introducing randomness into the integration path through random baseline sampling, thereby generating a pool of candidate attribution maps. The adaptability provided by multiple baselines enables RPI to select the most effective attribution map tailored to the specific evaluation metric. Through an extensive evaluation encompassing 11 explanation methods, 5 language models, and 4 datasets, our work establishes the superiority of RPI over current state-of-the-art methods across a diverse range of explanation metrics. These findings highlight the effectiveness of RPI as a machinery for explaining LMs.

6 Limitations and Future Work

While our RPI method has demonstrated its effectiveness in providing state-of-the-art results by sampling baselines from a Gaussian diffusion process, there exist certain limitations that merit consideration and avenues for future research.

Firstly, to enhance the variety of drawn baselines and, consequently, the resulting attribution maps, an exploration of additional baseline distributions is warranted. One potential avenue is to model the baseline distribution \mathcal{B} using a more diverse distribution, such as a mixture of distributions, as suggested in Section 3.

Another limitation lies in the non-adaptive nature of the sampling process in RPI. Adaptive sampling techniques can leverage information from already drawn baselines to intelligently decide the next region in space from which to draw baselines, thereby potentially improving performance on the metric of interest. Exploration-exploitation approaches, updating the baseline distribution in an online manner as sampling process evolves, could be explored to address this limitation.

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A Appendix

A.1 Layer ablation study

The evaluation results in Sec. 4.2 indicate that applying RPI solely to the last layer consistently yields state-of-the-art results. While this approach aligns with previous seminal explanation methods (Selvaraju et al., 2017; Caron et al., 2021) that predominantly utilize the final layer of the model for explanation generation, the general formulation of RPI, as described in Eq. 5, allows for the utilization of any arbitrary layer in the model and their combinations. Therefore, for the sake of completeness, in this section, we present an ablation study investigating the performance of RPI when applied to each individual layer in the model separately, as well as the benefits of aggregating attribution maps from multiple layers in the model.

To this end, we ablate over the layers in three different ways:

1. **Individual Layers:** We assess RPI’s performance when applied to each layer separately. This is achieved by setting J (Eq. 5) to a set containing the individual layer of interest each time.
2. **Top-down Aggregation:** RPI’s performance is evaluated when applied to a set of consecutive layers in a top-down manner. This involves combining the attribution maps produced starting from the top layer L (the last layer) downwards to layer $L - i$, with $i \in \{0, 1, \dots, 9\}$. Specifically, this is obtained by setting $J = \{L, L - 1, \dots, L - i\}$ in Eq. 5.
3. **Bottom-up Aggregation:** We assess RPI’s performance in a bottom-up manner, starting from the first layer and up to layer $L - i$. This is achieved by setting $J = 1, 2, \dots, L - i$ in Eq. 5.

Table 7 presents the results obtained based on the RTN dataset using an RTN finetuned BERT model (L stands for the last layer in the model). The Individual Layers section presents RPI results when applied to each individual layer $L - i$ separately, for $i \in \{0, 1, \dots, 11\}$. The Top-down Aggregation section presents RPI results for the combination of attribution maps produced by multiple consecutive layers in a top-down manner. Specifically, the row

associated with the layer $L - i$ corresponds to the application of Eq. 5 with $J = \{L, L - 1, \dots, L - i\}$. Conversely, in the Bottom-up Aggregation section, RPI is applied with $J = \{1, 2, \dots, L - i\}$ for the layer $L - i$.

It is important to clarify that the results in the ‘Top-down Aggregation’ and ‘Bottom-up Aggregation’ sections are derived from aggregating the attribution maps produced from each individual layer. Specifically, the RPI procedure was applied **once** for each individual layer, and the resulting attribution maps were then used for both top-down and bottom-up aggregations. Consequently, the results for full aggregation across all layers are identical for both top-down and bottom-up approaches (found in the first and last rows of the ‘Top-down Aggregation’ and ‘Bottom-up Aggregation’ sections, respectively). However, in all other cases, top-down aggregation outperforms bottom-up aggregation. For instance, aggregating the attribution maps from last 3 layers (corresponding to the row for $L - 2$ in the ‘Top-down Aggregation’ section) demonstrates superior performance compared to the aggregation of the attribution maps from the first 3 layers (corresponding to the row for $L - 7$ in the ‘Bottom-up Aggregation’ section).

Overall, the results in Tab. 7 indicate that performance tends to improve with deeper layers when applied individually, and as a result, it is preferred to aggregate attribution maps from the layers in a top-down manner.

A.2 Additional qualitative results

Table 8 showcases various RPI attributions obtained from multiple instances in the SST2 and EMR datasets, employing the RoBERTa model. The ‘Prediction’ column denotes the class with the highest prediction score by the model. In each example, the top three ranked words according to RPI attribution are highlighted in bold. Notably, the highlighted words exhibit semantic similarity to the predicted class, thereby offering a plausible explanation that supports the model’s prediction.

A.3 Evaluation metrics

For quantitative assessment of the explanation methods, we consider the following set of metrics:

1. **Log-Odds (LO)** (Shrikumar et al., 2017) score is defined as the average difference of the

| | Individual Layers | | | | | Bottom-up Aggregation | | | | | Top-down Aggregation | | | | |
|----------|-------------------|---------------|--------------|--------------|--------------|-----------------------|---------------|--------------|---------------|--------------|----------------------|---------------|--------------|---------------|--------------|
| | Suff↓ | LO↓ | Comp↑ | A-S↓ | A-C↑ | Suff↓ | LO↓ | Comp↑ | A-S↓ | A-C↑ | Suff↓ | LO↓ | Comp↑ | A-S↓ | A-C↑ |
| L | -0.018 | -2.583 | 0.610 | 0.005 | 0.309 | -0.021 | -3.357 | 0.725 | -0.010 | 0.369 | -0.018 | -2.583 | 0.610 | 0.005 | 0.309 |
| $L - 1$ | -0.019 | -2.573 | 0.609 | 0.003 | 0.314 | <u>-0.021</u> | <u>-3.301</u> | <u>0.718</u> | <u>-0.010</u> | <u>0.367</u> | -0.019 | -2.909 | 0.657 | -0.002 | 0.335 |
| $L - 2$ | <u>-0.019</u> | -2.675 | 0.622 | 0.002 | 0.319 | -0.021 | -3.233 | 0.713 | -0.009 | 0.363 | -0.020 | -3.108 | 0.686 | -0.004 | 0.350 |
| $L - 3$ | -0.018 | <u>-2.662</u> | <u>0.617</u> | <u>0.003</u> | <u>0.315</u> | -0.021 | -3.113 | 0.700 | -0.009 | 0.355 | -0.020 | -3.221 | 0.699 | -0.006 | 0.358 |
| $L - 4$ | -0.018 | -2.306 | 0.574 | 0.010 | 0.284 | -0.021 | -2.945 | 0.681 | -0.009 | 0.344 | -0.021 | -3.263 | 0.708 | -0.007 | 0.361 |
| $L - 5$ | -0.018 | -2.138 | 0.538 | 0.010 | 0.274 | -0.021 | -2.816 | 0.658 | -0.008 | 0.336 | -0.021 | -3.290 | 0.710 | -0.008 | 0.363 |
| $L - 6$ | -0.018 | -2.093 | 0.537 | 0.004 | 0.278 | -0.021 | -2.700 | 0.645 | -0.007 | 0.329 | -0.021 | -3.313 | 0.714 | -0.008 | 0.365 |
| $L - 7$ | -0.018 | -1.881 | 0.500 | 0.009 | 0.253 | -0.021 | -2.555 | 0.621 | -0.006 | 0.317 | -0.021 | -3.324 | 0.718 | -0.009 | 0.366 |
| $L - 8$ | -0.018 | -1.919 | 0.516 | 0.009 | 0.261 | -0.020 | -2.444 | 0.600 | -0.004 | 0.309 | -0.021 | -3.336 | 0.722 | -0.009 | 0.367 |
| $L - 9$ | -0.017 | -1.814 | 0.479 | 0.008 | 0.254 | -0.020 | -2.216 | 0.560 | -0.001 | 0.290 | -0.021 | -3.347 | 0.723 | -0.009 | 0.368 |
| $L - 10$ | -0.017 | -1.615 | 0.447 | 0.023 | 0.237 | -0.019 | -1.887 | 0.508 | 0.014 | 0.263 | <u>-0.021</u> | <u>-3.352</u> | <u>0.725</u> | <u>-0.010</u> | <u>0.369</u> |
| $L - 11$ | -0.013 | -1.421 | 0.411 | 0.047 | 0.216 | -0.013 | -1.421 | 0.411 | 0.047 | 0.216 | -0.021 | -3.357 | 0.725 | -0.010 | 0.369 |

Table 7: RPI layer ablation study using a finetuned version of BERT on the RTN dataset. L stands for the last layer in the model. The Individual Layers section presents RPI results when applied each individual layer in the model separately. This is achieved by setting J (Eq. 5) to a set containing the individual layer of interest each time. The Top-down Aggregation section presents RPI results when applied to multiple consecutive layers starting from the top layer L (the last layer) downwards. Specifically, the row associated with the layer $L - i$ corresponds to the application of RPI with $J = \{L, L - 1, \dots, L - i\}$. Conversely, in the Bottom-up Aggregation section, RPI is applied with $J = \{1, 2, \dots, L - i\}$ for the layer $L - i$. The results indicate that performance tends to improve with deeper layers when applied to a single layer, and therefore, it is preferred to aggregate attribution maps from the layers in a top-down manner.

Dataset Prediction Attribution

| | | |
|----------|---|---|
| EMR | Joy | i continue to feel so content about our decision to move here |
| | Fear | i have to take jenny in to be spayed so of course im feeling nervous and guilty |
| | Sadness | im feeling sentimental or in need of reassurance |
| | Fear | i was feeling a little fearful of trying to eat this damn thing |
| | Anger | i remember feeling so hellip furious with the shooter |
| | Anger | i just feel really violent right now |
| | Joy | i feel so tranquil right now its great |
| | Fear | i couldn t turn my head away even when i feel frightened |
| | Surprise | i feel so deeply shocked and saddened |
| | Fear | im feeling a combination of terrified and relieved |
| SST2 | Negative | first , for a movie that tries to be smart , it 's kinda dumb |
| | Negative | tedious norwegian offering which somehow snagged an oscar nomination |
| | Positive | the film retains ambiguities that make it well worth watching |
| | Negative | makes piecing the story together frustrating difficult |
| | Negative | doubtful this list less feature will win him any new viewers |
| | Positive | to emerge as an exquisite motion picture in its own right |
| | Positive | one of the most interesting writer /directors working today |
| Positive | would be forgettable if it were n't such a clever adaptation of the bard 's tragic play | |

Table 8: Examples of RPI attributions for multiple examples from the SST2 and EMR datasets (utilizing the RoBERTa model). The 'Prediction' column indicates the class associated with the highest prediction score by the model. In each example, the top three ranked words according to RPI attribution are marked in bold. The highlighted words demonstrate semantic similarity to the predicted class, thereby providing a reasonable explanation that supports the model's prediction.

negative logarithmic probabilities on the predicted class before and after masking the top $k\%$ words with <MASK> padding (Encoder-

based models) and <UNK> padding (Llama2). Lower scores are better. In this work, we used LO with $k = 20$.

2. Comprehensiveness (**Comp**) (DeYoung et al., 2020) score is defined as the average difference of the change in predicted class probability before and after removing the top $k\%$ features. Similar to Log-odds, this measures the influence of the top-attributed tokens on the model’s prediction. For a single example Comp is computed as:

$$p(y'|x_i) - p(y'|x_i^{(k)}),$$

where y' is the predicted class, x is the input sequence of tokens, and $x^{(k)}$ denotes the modified sequence with the top $k\%$ attributed tokens deleted from the sequence. Higher scores are better. In this work, we used Comp with $k = 20$.

3. Sufficiency (**Suff**) (DeYoung et al., 2020) score is defined as the average difference of the change in predicted class probability before and after keeping only the top $k\%$ tokens. This measures the adequacy of the top $k\%$ attributions for model’s prediction. It is defined in a similar fashion as comprehensiveness, except the $x^{(k)}$ is defined as the sequence containing only the top $k\%$ tokens. Lower scores are better. In this work, we used Suff with $k = 20$.
4. Area Over the Perturbation Curves (AOPC): AOPC-Sufficiency (**A-S**) and AOPC-Comprehensiveness (**A-C**) (DeYoung et al., 2020) - are the average differences of the change in predicted class probability before and after keeping and removing the top $k\%$ tokens for Sufficiency and Comprehensiveness, respectively:

$$\text{AOPC-S} = \frac{1}{|B|} \sum_{k \in B} \text{Suff}(k),$$

$$\text{AOPC-C} = \frac{1}{|B|} \sum_{k \in B} \text{Comp}(k).$$

Here, we evaluate Comp and Suff for 5 different values of k , setting $B = \{1, 5, 10, 20, 50\}$ as suggested by (DeYoung et al., 2020). A-S and A-C measure how well a specific token ordering is scored under a model from two complementary perspectives and across the k

axis.

A.4 LLM prompts

This section outlines the prompts used by the Llama2 and Mistral models for each dataset in a few-shot context. Utilizing these prompts led to classification accuracy exceeding 90% for the SST2 and RTN tasks, which is also true for the LoRA-based finetuned models for the AGN and EMR tasks. It is noteworthy that in a zero-shot mode, the results experience a significant degradation.

A.4.1 SST2 prompt

Classify the sentiment of sentences. for each sentence the label is positive (P) or negative (N)

Text: hide new secretions from the parental units
Label:N

Text: the greatest musicians
Label:P

Text:are more deeply thought through than in most ‘right-thinking’ films
Label:P

Text: on the worst revenge-of-the-nerds clichés the filmmakers could dredge up
Label:0

Text:[text]
Label:

A.4.2 RTN prompt

Classify the sentiment of sentences. for each sentence the label is positive (P) or negative (N)

Text: the film desperately sinks further and further into comedy futility.
Label:N

Text: if you sometimes like to go to the movies to have fun , wasabi is a good place to start .
Label:P

Text: plays like the old disease-of-the-week small-screen melodramas .

Label:N

Text: hip-hop has a history , and it's a metaphor
for this love story .

Label:P

Text: spiderman rocks

Label:P

Text:so exaggerated and broad that it comes
off as annoying rather than charming .

Label:N

Text:[text]

Label: