Rationalizing Transformer Predictions via End-To-End Differentiable Self-Training

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Abstract

We propose an end-to-end differentiable training paradigm for stable training of a rationalized transformer classifier. Our approach results in a single model that simultaneously classifies a sample and scores input tokens based on their relevance to the classification. To this end, we build on the widely-used three-playergame for training rationalized models, which typically relies on training a rationale selector, a classifier and a complement classifier. We simplify this approach by making a single model fulfill all three roles, leading to a more efficient training paradigm that is not susceptible to the common training instabilities that plague existing approaches. Further, we extend this paradigm to produce class-wise rationales while incorporating recent advances in parameterizing and regularizing the resulting rationales, thus leading to substantially improved and state-of-the-art alignment with human annotations without any explicit supervision.

1 Introduction

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Neural networks are increasingly prevalent across a wide range of applications, driving significant advancements in fields such as natural language processing, computer vision, and beyond. Due to the black-box nature of these networks, this widespread use comes with an increased demand for interpretability (Lyu et al., 2024), as understanding the basis for the decisions made by these models is crucial for their reliable and ethical deployment. This need has become especially clear with the increasing use of notoriously uninterpretable large language models, which have the potential to quickly lose a user's trust after only few confidently incorrect predictions (Dhuliawala et al., 2023).

One possible mitigation is the use of encoderonly models, which lend themselves more readily to classical interpretability approaches designed for general neural network classifiers while still providing state-of-the-art performance due to continuous improvements in model structure (He et al., 2021, 2023) and training paradigms (Zhang et al., 2023).

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While a variety of explainability methods exist, that usually assign scores to input tokens indicating their importance for a classification (Sun et al., 2021), these methods often suffer from several drawbacks, including high computational cost, difficult-to-interpret explanations, and potentially even unfaithful representations of the model's decision-making process. In this study, we close this gap by developing a rationalized transformer predictor that generates faithful and interpretable explanations in addition to its decisions within the same forward pass.

As a foundation for our approach, we build upon the existing and commonly used three-player game proposed by Yu et al. (2019). In this framework, a selector model chooses a subset of the input as rationale, while a predictor and a complement predictor model are trained to infer the correct label from either the tokens included in the rationale or the tokens not included in the rationale, respectively. The selector model is then trained to maximally aid the predictor in predicting the correct label while preventing the complement predictor from doing the same, thus ensuring that all tokens indicative of the correct label are included in the rationale.

While the general three-player game is sensible, the actual realizations that are proposed often have several limitations, including being not end-to-end differentiable due to a stochastic sampling process in the forward pass, showing interlocking dynamics that might prevent convergence to a suitable solution, and having no guarantee of providing a rationale that actually explains the prediction (compare Section 2.3 for a more detailed discussion).

For this reason, we propose a new take on this three-player game that is not susceptible to these drawbacks. We achieve this by making use of a single unified model that is trained as a standard classifier on the complete unaltered input, while

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simultaneously predicting class-wise importance scores for each input token in the same forward pass, which are then trained using self-training to mark spans that the model itself considers important for the specific class.

Our proposed rationalized transformer predictor (RTP) simplifies and enhances the common three-player structure in several ways, including 1) using only a single model to fulfill all three roles of the three-player game, thus enabling classification and rationale prediction in a single forward pass 2) training the rationales to explain the predictor, but avoiding training the predictor on the rationales, which ensures that the rationales faithfully explain the predictions 3) creating rationalized inputs in continuous fashion to enable fully differentiable training and avoid sampling 4) creating class-wise rationales and 5) using a parameterization that maximizes similarity with human rationale annotations.

We evaluate our method on two benchmarks for explainable AI and compare it with existing post-hoc explanation methods as well as methods leveraging standard multi-player procedures. We show that our method achieves state-of-the-art performance on both tasks, demonstrating previously unseen alignment with human rationales in combination with high rationale faithfulness.

2 Background

2.1 **Post-Hoc Rationalization**

Since neural networks are black-box models, the ever-increasing use of such model in research and industry has led to a strong demand for methods that reliably explain neural network classifications. To this end, a variety of approaches have been proposed, many of which are designed to create posthoc explanations for an already trained classifier. These methods rely on a variety of mechanisms, 119 including 1) making use of the models gradients 120 at different inputs to obtain importance scores (Simonyan et al., 2013; Sundararajan et al., 2017) 2) 122 quantifying the influence of individual input ele-123 ments by observing the effect of input perturbations 124 (Castro et al., 2009; Zeiler and Fergus, 2014; Zhou 125 et al., 2014; Petsiuk et al., 2018) 3) fitting inter-126 pretable models to neural-network outputs (Ribeiro 128 et al., 2016) 4) developing backpropagation-like procedures to propagate importance information 129 from the model output to the input features (Zeiler 130 and Fergus, 2014; Springenberg et al., 2015; Bach et al., 2015; Shrikumar et al., 2017; Chefer et al., 132

2021a,b) 5) performing input-optimization to create an altered input that only retains the information important for the classification (Brinner and Zarrieß, 2023).

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Rationalized Classification 2.2

Due to the inherent difficulty of creating post-hoc explanations for classifiers that were never designed to be explainable, rationalized predictors have been proposed that are explicitly trained to perform the original task while simultaneously providing a rationale for the prediction in a single forward pass. Lei et al. (2016) were the first to propose a two-player game for textual inputs, involving a rationale selector model and a classifier model. The rationale selector assigns a probability to each input word, indicating its likelihood of belonging to the rationale, so that a discrete rationale can be sampled from this distribution. The classifier then uses only the rationale to make its classification, thus ensuring that the selected words were responsible for the classification. During training, the classifier is trained as usual to predict the correct label from a sampled rationale, while the rationale selector is trained to produce rationales that aid the classifier in making the correct predictions, ensuring that words indicative of the correct class are selected.

2.3 **Common Issues of Rationalized Classifiers**

While the general training paradigm of the twoplayer game is sensible, several issues affect the training, performance and faithfulness of the rationales:

- 1. Stochastic Sampling: Training requires stochastic sampling of rationales, meaning that gradients can only be estimated using methods like REINFORCE (Williams, 1992), which are generally less stable and slow to convergence.
- 2. Class-Independent Rationales: A single rationale is predicted regardless of the sample's class. In case a sample belongs to multiple classes, it is not possible to identify which part of the input is indicative of a specific class.
- 3. Interlocking Dynamics: Interlocking dynamics might lead to degenerate solutions, for example, if the rationale predictor adapts too quickly to the noisy rationales that are produced by the randomly initialized rationale selector or vice versa (Yu et al., 2021).

4. **Dominant Selector**: The training paradigm enforces rationales that persuade the classifier to predict a label that the predictor deemed correct, which does not necessarily correspond to faithful explanations of the actual reasoning process (Jacovi and Goldberg, 2021). In extreme cases, the rationale generator might simply encode the correct classification in the rationale (e.g., by selecting a specific kind of token), so that the classifier does not perform any significant reasoning itself.

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- 5. **Mismatch with Human Annotations**: Often, rationales are most-useful if they resemble rationales provided by human annotators. Despite regularizers designed to enforce the selection of longer, consecutive spans of text, models often struggle to select spans that match human annotations, since overly strong regularization often overpowers the weak gradient signal created by REINFORCE, leading to degenerate solutions (e.g., selecting no tokens or all tokens).
- 6. **Degraded Classification Performance**: The actual classification performance often degrades compared to standard classifiers (Jacovi and Goldberg, 2021).

Several approaches have been proposed to modify or extend the two-player game to address these issues. Yu et al. (2019) extended this paradigm into a three-player game by introducing a complement predictor that is trained to predict the correct label from all words not included in the rationale. The rationale selector is then trained to prevent the complement predictor from identifying the correct class, thus ensuring that all words indicative of the correct class are selected as rationale, addressing issue 3 and (in part) issue 4. Chang et al. (2019) propose the CAR framework that uses two encoders and one decoder per class to generate class-wise and potentially counterfactual) rationales, solving issues 2, 3 and (in part) 4. They also use the straight-through gradient estimator (Bengio et al., 2013) instead of using REINFORCE, which addresses issue 1. Liu et al. (2023) make use of multiple generators to mitigate issue 3, while the A2R method (Yu et al., 2021) addresses the same issue by introducing a separate predictor that uses a soft selection of inputs instead of binary thresholding. To our knowledge, our proposed method for training a rationalized classifier is the only one to address all of the issues discussed above.

3 Method

We propose a new method for end-to-end differentiable training of a rationalized transformer predictor (RTP). In the following, plain letters (e.g., x) denote scalars, while bold letters (e.g., x) denote vectors or tensors. We assume a text classification problem with label set \mathcal{Y} , and a training set consisting of texts $\mathbf{x}_0, ..., \mathbf{x}_n$ with corresponding ground truth vectors $\mathbf{y}_0, ..., \mathbf{y}_n$.

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3.1 Concept

The RTP relies on a single model that, in one forward pass, produces both a classification output and class-wise importance scores for each token, denoting how indicative each token is of the respective class. The classification component is trained as a standard classifier, while the token-wise rationales are trained by creating altered inputs that only retain the important information for each individual class. The quality of these altered inputs (and therefore the quality of the rationales) is judged by the model itself by passing them through the model and observing its classification output. Through this end-to-end differentiable procedure, the rationales are optimized to faithfully explain the model predictions.

3.2 Model Structure

The basis of our method is a single model M, that, given an input text **x**, simultaneously predicts class probabilities $\tilde{\mathbf{y}}$, as well as a mask tensor **m**:

$$\tilde{\mathbf{y}}, \mathbf{m} = M(\mathbf{x}) \tag{1}$$

with the mask **m** being the rationale for the classification output $\tilde{\mathbf{y}}$. Notably, **m** consists of $|\mathcal{Y}|$ individual vectors $\mathbf{m}^0, ..., \mathbf{m}^{|\mathcal{Y}|}$ that constitute individual rationales for each class $c \in \mathcal{Y}$, with each \mathbf{m}^c being a vector containing a mask value m_i^c in the range 0 to 1 for each input token x_i , indicating its influenc on the predicted likelihood of class c. In practice, the basis for classification output $\tilde{\mathbf{y}}$ will be the *CLS*-token embedding of the transformer classifier, while the mask values **m** will be calculated from the predicted outputs for each token.

3.3 Mask Parameterization

In this section, we will discuss the parameterization that transforms token-wise neural network outputs into a smooth mask. The RTP outputs a mask for each individual class, but since mask calculations for individual classes are independent of each other,



Figure 1: An exemplary output of the RTP for a positive review from the movie reviews dataset.

we will look at the mask \mathbf{m}^c for a single class c, denoted as \mathbf{m} for simplicity.

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A simple mask parameterization would predict a logit l_i for each token x_i and define $m_i = \sigma(l_i)$. Even with regularizers that enforce smooth mask selections, this approach often fails to select long spans of text as rationales, which would be desirable for matching human annotations. For this reason, we opted for the mask parameterization proposed by Brinner and Zarrieß (2023) that explicitly enforces the prediction of longer spans of text as rationales by letting neighboring mask values influence each other.

In this parameterization, the model outputs two values w_i and σ_i for each word x_i . w_i is mainly responsible for determining the mask value of word x_i , while σ_i determines the influence of w_i on the mask values of neighboring words. Introducing regularizers to enforce large values for σ_i then leads to smooth masks. The mathematical formulation of the parameterization is as follows:

$$w_{i \to j} = w_i \cdot \exp\left(-\frac{d(i,j)^2}{\sigma_i}\right) \tag{2}$$

$$m_j = \text{sigmoid}(\sum_i w_{i \to j})$$
 (3)

Here, d(i, j) denotes the distance between two words x_i and x_j and $w_{i \rightarrow j}$ is the influence of w_i on the mask value of word j. m_j is then calculated by applying the sigmoid to the sum of all influence values, resulting in the mask **m** for the specific class at hand. Predicting masks $\mathbf{m}^0, ..., \mathbf{m}^{|\mathcal{Y}|}$ for each class will simply be done by predicting individual outputs \mathbf{w}^c and $\boldsymbol{\sigma}^c$ for each class c and performing the calculations independently.

3.4 Model Training

Given a sample (\mathbf{x}, \mathbf{y}) , the classification capabilities of model M are trained like a standard neural network classifier by performing a prediction and applying a loss function like cross-entropy loss to the predicted output. In contrast to other rationalized models, our training paradigm therefore trains the classifier on the unaltered input, not on a masked version that might remove crucial information. To train the rationale predictions (i.e., the masks **m**), we use these masks to create two altered inputs \mathbf{x}^c and $\overline{\mathbf{x}}^c$ for each ground-truth class c, with input \mathbf{x}^c retaining all information that is indicative of class c according to mask \mathbf{m}^c , while $\overline{\mathbf{x}}^c$ is the complement input that removes all information specified by mask \mathbf{m}^c :

$$\mathbf{x}^c = \mathbf{m}^c \cdot \mathbf{x} + (1 - \mathbf{m}^c) \cdot b \tag{4}$$

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$$\overline{\mathbf{x}}^c = (1 - \mathbf{m}^c) \cdot \mathbf{x} + \mathbf{m}^c \cdot b \tag{5}$$

Here, *b* denotes an uninformative background (e.g., *PAD*-token embeddings). Notably, the mask **m** is applied in continuous fashion to **x** and *b*, meaning that embeddings for words are linearly blended towards uninformative embeddings according to **m**. In contrast to sampling of a discrete mask, this ensures full differentiability and was proven to have the desired effect of gradual removal of information by Brinner and Zarrieß (2023).

The rationalized inputs are then fed back into the same model M and are trained to allow it to predict the correct label from \mathbf{x}^c , but not from $\overline{\mathbf{x}}^c$, meaning that all information indicative of class c is contained in the rationale (thus enforcing rationale comprehensiveness). The loss formulations used are the following:

$$\mathcal{L}^c = \mathbf{C}\mathbf{E}(M(\mathbf{x}^c), \mathbf{y}) \tag{6}$$

$$\mathcal{L}^{\overline{c}} = \operatorname{relu}(M(\overline{\mathbf{x}}^c)[c] - \alpha) \tag{7}$$

where **CE** denotes the cross-entropy loss, $M(\mathbf{x})[c]$ denotes the predicted probability of class c and α is a hyperparameter ensuring that the model is not required to drive the probability of class c for input $\overline{\mathbf{x}}^c$ to 0, since driving it to a small value is sufficient. Importantly, the model M is only trained with respect to the first forward pass that produces the rationales, and is therefore not updated to improve classification on the altered inputs \mathbf{x}^c and $\overline{\mathbf{x}}^c$. This ensures that the classification performance in not influenced, and that the rationales actually explain the classification instead of dictating it. The final optimization problem looks as follows:

$$\underset{M}{\operatorname{arg\,min}} \quad \mathbf{CE}(M(\mathbf{x}), \mathbf{y}) + \sum_{c \in \mathbf{y}} \left[\mathcal{L}^{c} + \mathcal{L}^{\overline{c}} \right] \\ + \Omega_{\lambda} + \Omega_{\sigma}$$
(8)

where $c \in \mathbf{y}$ indicates summing over all ground-361 truth labels and Ω_{λ} and Ω_{σ} denote regularizers that 362 enforce sparsity and smoothness of the rationales, respectively. Details on these regularizers and further details on the general objective are available in Appendix A.3.

3.5 Advantages

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Our proposed scheme solves all issues discussed in Section 2.3, and is (to our knowledge) the only method to do so. The main advantages lie in the fully differentiable formulation that does not require sampling and gradient approximation, the fact that class-wise rationales are created, and especially in the fact that the classifier is trained on the 374 unaltered inputs instead of on the rationalized vari-375 ants. This last point ensures that the rationales do 376 not dictate the classification result, but instead explain the actual classification made by the classifier. 378 It also means that no degradation is classification performance is to be expected.

Experiments 4

We evaluate our method with regards to matching human evidence annotations for text classifications, as well as with regards to the faithfulness of the explanations with regards to the classifier. For details regarding the model and the training and prediction procedures, see Appendix A.

4.1 Datasets

In our evaluation, we use two text classification datasets with span-level evidence annotations, each posing different challenges. The first is the movie review dataset (Zaidan et al., 2007), containing 2000 reviews with sentiment labels (positive or negative) and span-level evidence annotations. For this dataset, DeYoung et al. (2020) provided more comprehensive rationales for the test split, which we use in our evaluation. Since class labels are mutually exclusive, this dataset allows models to perform optimally even without class-wise rationales. Additionally, this dataset enables optimal assessment of agreement between predicted rationales and human annotations, since the simplicity of the classification task eliminates the lack of understanding of the inputs as a cause for mismatches.

As for a more challenging classification task, we use the INAS dataset (Brinner et al., 2022), consisting of 954 scientific paper titles and abstracts from the domain of invasion biology together with labels indicating which hypothesis (from a set of 10 common hypotheses in the field) is addressed in each paper. In a subsequent study, Brinner et al. (2024) provided span-level evidence annotations for 750 of the samples. Since some samples have multiple correct labels, optimal performance on this dataset requires class-wise rationalization. Additionally, the more challenging nature of the classification task can highlight degraded classification performance of rationalized models.

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4.2 Evaluation Metrics

We evaluate the consistency with human annotations on token-level and span-level as done in (Brinner et al., 2024), and evaluate the faithfulness of rationales with respect to the classifier as done in (Brinner and Zarrieß, 2023).

Token-Level Evaluation To evaluate agreement with human rationales at the token level, we use the area under the precision-recall curve (AUC-PR). We also assess the token-level F1 score (Token-F1), which requires binary predictions. This is done by selecting the highest-scoring p percent of tokens as positive predictions, calculating the standard F1 score, and averaging over 19 values of p (5, 10, ..., 95). For a better absolute assessment of prediction quality, we use the discrete token-level F1 score (D-Token-F1), where the top k tokens (matching the number in the ground-truth annotation) are treated as the rationale and evaluated with the F1 score.

Span-Level Evaluation We also evaluate the quality of predicted spans of text, defined as consecutive words selected as part of the rationale after binary thresholding. The span-level IoU-F1 score (IoU-F1) is calculated by determining spans in both the binary rationale prediction and the ground-truth annotation, calculating the IoU for all span pairs, and selecting the maximum IoU for each predicted and annotated span. IoU-precision and IoU-recall are then defined as the averages of these maximum IoU values for predicted and ground-truth spans, respectively. The holistic IoU-F1 score is then obtained by averaging over the same 19 discrete token selections used for the token-level F1 score. The discrete IoU-F1 score (D-IoU-F1) is again calculated by selecting the top-scoring tokens to match the number in the ground-truth annotation.

Faithfulness Evaluation We evaluate faithfulness using scores for sufficiency and comprehensiveness of the predicted rationales. The sufficiency score measures the model's ability to predict the correct label using only the highest-scoring words

Method	Clf-F1	AUC-PR	Token-F1	D-Token-F1	IoU-F1	D-IoU-F1	Suff. \downarrow	Comp.↑	Perf.
Random	-	0.220	0.255	0.222	0.067	0.003	0.194	0.191	0.289
Supervised	0.730	0.557	0.406	0.509	0.231	0.257	0.005	0.396	1.028
MaRC	0.748	0.366	<u>0.336</u>	0.351	<u>0.219</u>	0.178	-0.002	0.396	0.953
Occlusion	0.748	0.307	0.277	0.294	0.145	0.071	0.020	0.315	0.717
Int. Grads	0.748	0.315	0.302	0.318	0.087	0.013	-0.017	0.465	0.871
LIME	0.748	0.272	0.280	0.273	0.082	0.007	0.039	0.357	0.680
Shapley	0.748	0.309	0.301	0.320	0.084	0.009	-0.083	0.515	0.983
L2E-MaRC	0.748	<u>0.431</u>	0.359	0.402	0.174	0.131	0.020	0.427	0.940
2-Player	0.675	0.272	0.286	0.270	0.085	0.007	-0.050	0.303	0.724
3-Player	0.722	0.287	0.296	0.286	0.080	0.004	0.023	0.403	0.756
CAR	-	0.314	0.281	0.280	0.184	0.133	-	-	-
A2R	0.686	0.268	0.287	0.264	0.084	0.008	0.122	0.282	0.531
A2R-Noise	0.618	0.271	0.285	0.262	0.087	0.011	0.072	0.198	0.498
RTP	0.710	0.436	0.359	0.415	0.220	0.203	0.066	0.565	1.078

Table 1: Results on the INAS dataset, divided into groups of standard-baselines, post-hoc explainability methods and rationalized neural networks. Best scores per metric are bold, second best are underlined.

in the rationale. A lower sufficiency score indicates that fewer tokens are needed for a correct prediction, thus indicating a more faithful rationale:

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sufficiency
$$(x, r) = \frac{1}{19} \sum_{i=1}^{19} M(x) - M(r_i)$$
 (9)

The comprehensiveness score is higher if removing the highest-scoring words according to the rationale quickly degrades the model's predictions, again indicating faithful rationales:

$$comp(x, r) = \frac{1}{19} \sum_{i=1}^{19} M(x) - M(x \setminus r_i) \quad (10)$$

In these equations, x denotes the input sample, r_i denotes the $(i \cdot 5)\%$ of input tokens with the highest scores according to the rationale, $x \setminus r_i$ denotes the input x with the tokens from r_i removed, and M(x)denotes the probability that model M assigns to the correct class given input x. To avoid relying on a single threshold, these scores are calculated by summing over different percentages of rationale tokens used or removed, respectively.

Overall Performance Ideally, a model should produce rationales that both agree with human rationales and demonstrate faithfulness. We therefore provide an overall performance score (*Perf.*) that sums over the Token-F1, IoU-F1, comprehensiveness and negative sufficiency scores, thus assessing agreement and faithfulness comprehensively.

4.3 Baseline Methods

We compare our rationalized transformer predictor (RTP) against other rationalized classifiers, which are a two-player game as proposed by Lei et al. (2016), a three-player structure with complement predictor (Yu et al., 2019), the CAR framework for class-wise rationale generation (Chang et al., 2019), and the A2R method (Yu et al., 2021) as well as an extension to it using noise injection (Storek et al., 2023). We also compare post-hoc explainability methods that are applied to a standard classifier, which includes MaRC (Brinner and Zarrieß, 2023), Occlusion (Zeiler and Fergus, 2014), Integrated Gradients (Sundararajan et al., 2017), LIME (Ribeiro et al., 2016), Shapley value sampling (Castro et al., 2009), as well as a neural network predictor trained on MaRC rationales (L2E-MaRC, Situ et al. (2021)). Finally, we report results for a supervised model trained on rationale annotations and a random predictor as additional baselines. For a more detailed overview, see Appendix A.1.

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5 Results

The results for the evaluation on the movie review dataset and the INAS dataset are displayed in Table 2 and Table 1, respectively. Exemplary predictions are displayed in Figure 1, with further examples being included in Appendix B.

5.1 Classification Performance

On the INAS dataset, our RTP method ranks among the best-performing rationalized neural networks, although all rationalized models show slightly worse classification performance compared to a standard classifier (used by the post-hoc methods). We do not attribute this to a generally decreased classification ability of the rationalized classifiers, since we selected the best-performing version of each model with respect to rationale-predictions

Method	Clf-F1	AUC-PR	Token-F1	D-Token-F1	IoU-F1	D-IoU-F1	Suff. \downarrow	Comp.↑	Perf.
Random	-	0.316	0.326	0.312	0.061	0.002	0.227	0.238	0.398
Supervised	0.980	0.670	0.514	0.626	0.144	0.169	0.001	0.638	1.295
MaRC	<u>0.965</u>	0.428	0.404	0.423	0.181	0.118	0.036	0.478	1.027
Occlusion	<u>0.965</u>	0.409	0.367	0.377	0.151	0.079	-0.021	0.569	1.108
Int. Grads	0.965	0.376	0.358	0.371	0.067	0.009	0.049	0.484	0.860
LIME	<u>0.965</u>	0.379	0.361	0.369	0.076	0.014	0.005	0.603	1.035
Shapley	0.965	0.442	0.390	0.426	0.082	0.020	-0.029	0.827	1.328
L2E-MaRC	0.965	0.565	0.460	0.534	0.126	0.104	-0.016	0.652	1.254
2-Player	0.930	0.516	0.449	0.508	0.113	0.066	-0.024	0.210	0.796
3-Player	0.955	0.458	0.422	0.465	0.089	0.023	0.003	0.354	0.862
CAR	-	0.384	0.364	0.376	0.078	0.013	-	-	-
A2R	0.955	0.474	0.433	0.486	0.111	0.046	0.109	0.320	0.755
A2R-Noise	0.950	0.483	0.440	0.492	0.107	0.044	0.005	0.338	0.880
RTP	0.975	<u>0.558</u>	<u>0.458</u>	0.527	0.192	0.177	-0.006	<u>0.803</u>	1.459

Table 2: Results on the movie reviews dataset, divided into groups of standard-baselines, post-hoc explainability methods and rationalized neural networks. Best scores per metric are bold, second best are underlined.

on the validation set, not with respect to classification performance. Additionally, this task shows a high variance between training runs (Brinner et al., 2022). Results on the movie review dataset are similar, with most rationalized classifiers performing slightly worse than the standard classifier. Notably, the RTP even outperforms the baseline, which we again attribute to variance between training runs.

5.2 Token-Level Performance

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For token-level rationale evaluations on the INAS dataset, our RTP method outperforms others in AUC-PR, token-F1, and discrete token-F1 scores. Only the L2E-Marc method, which is a neural network trained to predict rationales created by the MaRC method, comes close to or matches the RTP. A discussion of the superior performance of these exact two methods is done in Section 6. Especially the ability to predict class-wise rationales benefits the RTP and the post-hoc methods on this dataset compared to the other rationalized neural networks, since only the CAR method possesses this ability among them. This can also be seen by noticing the much better performance of these rationalized networks on the movie review dataset, since on this task the ability to predict class-wise rationales is irrelevant, thus reducing the gap to the RTP and making them surpass most post-hoc methods. Generally, the supervised baseline outperforms all methods with regards to token-level predictions, which is to be expected considering that the weakly supervised methods were never explicitly told what to predict. However, the RTP comes rather close to the supervised baseline in many metrics, indicating that in the absence of ground-truth rationales for

training, using the weakly supervised scheme can be an effective alternative.

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5.3 Span-Level Performance

Our RTP method is consistently the best performing method with regards to the IoU-F1 and the discrete IoU-F1 scores. Compared to the other rationalized methods this is to be expected, since the RTP has been explicitly designed to extract longer spans of text as rationales. In contrast, other rationalized predictors often rely on a total variation regularizer in their optimization objective, which we found to be ineffective since increasing it's strength quickly leads to degenerate solutions with either all or none of the words being selected. This highlights the importance of using the MaRC mask parameterization that reliably leads to the desired results. Notably, the RTP comes close to the supervised method on the INAS dataset without any supervision regarding the usual form of human annotations. On the movie review dataset, the RTP even outperforms the supervised method due to the rationales from the test set being more extensive, thus causing a mismatch between training and test data distributions. This shows, that even if slightly inaccurate training data is available for a given task, using a weakly supervised method instead might be preferable.

5.4 Faithfulness Results

Our RTP method achieves competitive sufficiency scores and state-of-the-art comprehensiveness scores. We found that assigning high scores to few important words distributed throughout the whole input is a great strategy for achieving high sufficiency, since the model can quickly recognize the correct label from these few highly indicative words. Our RTP model still performs well despite being explicitly discouraged from pursuing this strategy, indicating that our optimization objective is reasonable for generating faithful rationales.

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For comprehensiveness, the RTP attains stateof-the-art results on the INAS dataset and nearly matches the Shapley value sampling method on the movie reviews dataset, with both methods outperforming all other contenders by a large margin. Good faithfulness scores for Shapley value sampling are expected, though, since its objective for scoring input tokens aligns closely with the evaluation measures for faithfulness.

Overall, our RTP method compares favourably to other rationalized neural networks, since it optimizes its rationales to actually explain the classification, while other methods suffer from issues like a dominant predictor that already dictates a specific label, and additionally train the predictor on the rationales, which leads to a constant mismatch between the current predictor and the predictor that the rationales have been trained to explain.

Another important insight is, that post-hoc explanation methods do not offer an advantage over the rationales generated by the RTP. Considering, that post-hoc explainers outperform other rationalized networks with respect to faithfulness of the explanations, our method is the first all-in-one method that offers both predictions and rationales with state-ofthe-art faithfulness in a single forward pass.

5.5 Overall Performance

As discussed, the RTP achieves state-of-the-art results in agreement with human rationales and rationale faithfulness, resulting in dominant scores for overall performance (*Perf.*) on both tasks. In comparison, other rationalized neural networks fall significantly short, with only few post-hoc methods coming somewhat close. These methods have the downside of a substantially higher computational cost in producing a rationale, with, for example, MaRC and Shapley value sampling requiring hundreds of forward passes to create a single rationale.

6 Discussion

The RTP model demonstrated strong performance across all evaluated metrics. Comparing it specifically to the MaRC method, it outperformed it in every metric related to measuring agreement with human annotations and most faithfulness met-640 rics. This is notable since the RTP can be seen 641 as a neural network parameterized version of the 642 MaRC approach, which originally optimized mask 643 parameters for each sample individually instead 644 of training a neural network to directly predict 645 them from the input. Another well-performing 646 method, especially with regards to token-level eval-647 uation, is the L2E-MaRC method. The L2E frame-648 work (Situ et al., 2021) trains a neural network 649 on pre-calculated rationales created by a post-hoc 650 explainer. Even though it only saw rationales pro-651 duced by the MaRC method, it manages to out-652 perform it on all metrics measuring token-level 653 agreement with human rationales. These two re-654 sults indicate, that training to explain many differ-655 ent samples leads to better generalization, which 656 we attribute to reduced overfitting to one specific 657 input. This effect is crucial for the RTP, since it per-658 forms input optimization with respect to specific 659 neural network outputs, which has been shown to 660 generally lead to unexpected and uninterpretable ar-661 tifacts (Simonyan et al., 2013). The MaRC method 662 successfully mitigated this issue by combining con-663 strained optimization with heavy regularization, but 664 artifacts (i.e., unexpected spans included in the ra-665 tionale) are still to be expected. In the case of the 666 RTP, training on many samples further reduces this 667 issue, since these unwanted gradient signals will 668 generally not match between different samples, so 669 that the neural network mainly adapts to the wanted 670 signal that is consistent within larger parts of the 671 training set, and that corresponds to features that 672 are generally indicative of the respective class. 673

7 Conclusion

We presented a new method for training a rationalized transformer predictor and demonstrated its strong performance on two natural language processing benchmarks. Since our proposed training scheme is not invasive to the general training process and does not produce significant overhead during prediction, we believe that this approach has the potential to facilitate wider adoption and availability of rationalized predictors. Given that transformers are widely used in other modalities (Dosovitskiy et al., 2021; Verma and Berger, 2021), we hypothesise that our approach can be extended to these modalities and potentially lead to results of similar quality.

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8 Limitations

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While our method for rationalization generally does not interfere with the training of the prediction module and does not produce notable overhead during prediction, it nevertheless increases the computational cost of model training due to a second forward pass through the model, as well as through more training epochs being required due to slower convergence of rationale training compared to the classification component.

Additionally, the exact form of the produced rationales depends on the models inner working, so that generally a high overlap with human rationales is not guaranteed in cases where the model's reasoning and human reasoning differ.

Finally, while having access to word-level rationale scores is generally helpful, this does not equate to a complete description of the model's inner workings and the actual reasoning process, which most likely is impossible to represent in such a simple form.

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A Experimental Details

The code for our experiments is available at *Link* will be added in final version of the paper.

A.1 Baseline Methods

We evaluate our rationalized transformer predictor against a variety of baseline methods that pursuit different strategies for rationalizing predictions. This section provides a general overview, with many model and training details being discussed in Appendix A.2. The first group are rationalized neural networks, that learn to create rationales from sample-level labels alone. We evaluate the performance of the following methods:

- **2-Player**: A two-player structure using a rationale extractor and a predictor as proposed by Lei et al. (2016). We used an own implementation, since the original work did not use transformers.
- **3-Player**: A three-player structure using a rationale extractor, a predictor and a complement predictor as proposed by Yu et al. (2019). We used an own implementation, since the original work did not use transformers.
- **CAR**: The CAR framework for creating classwise rationales (Chang et al., 2019). We use an own implementation, since the original

work did not use transformers. Additionally, we use more extensive parameter sharing, as the original work use a separate rationale predictor for each class, which is impracticable especially for the 10-class classification problem on the INAS dataset. Therefore, a single BERT model predicts rationales for each class at the same time, while a second BERT model acts as the single predictor.

- A2R: The A2R framework as proposed by (Yu et al., 2021). We use the implementation of (Storek et al., 2023), who created an implementation relying on BERT models, which, according to their evaluation, outperformed the original implementation that relies on GRUs.
- **A2R-Noise**: The A2R framework with additional noise injection as proposed by (Storek et al., 2023). We use the implementation provided by the original study.

We also evaluated a variety of post-hoc explanation methods:

- MaRC: The MaRC method as proposed by (Brinner and Zarrieß, 2023). We use the updated weight regularizer proposed by (Brinner et al., 2024).
- Occlusion: The occlusion method as proposed by Zeiler and Fergus (2014). We chose to mask slightly larger spans of 5 tokens as this produced smoother masks which resulted in higher IoU F1 scores. We use the implementation by Kokhlikyan et al. (2020).
- **Int. Grads**: The integrated gradients method (Sundararajan et al., 2017). We use the implementation by (Kokhlikyan et al., 2020).
- LIME: The LIME method (Ribeiro et al., 2016). We train a linear classifier on scores from 50 function evaluations. In each evaluation, 5 13% of tokens are selected and the thee tokens starting from the chosen token are removed as input perturbation. We use the implementation by (Kokhlikyan et al., 2020).
- **Shapley**: Shapley value sampling (Castro et al., 2009). We perform 25 feature permutations per sample, and use the implementation by (Kokhlikyan et al., 2020).
- L2E-MaRC: The L2E framework (Situ et al., 2021). We use the rationales created by the MaRC method on the training samples. We discretize the rationales into 5 bins and train

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1010a classifier on this dataset. For scoring, we1011predict the bin-probabilities for each word,1012multiply them by the bin-means and sum over1013the resulting values to get a single, continuous1014score for each word.

We also evaluate two further baselines: A random baseline that predicts random scores for each input token, and a supervised method that is trained to perform a binary prediction on each individual token from the input.

A.2 Model and Training Details

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Base Models For the movie review experiment, we use bert-base-uncased (Devlin et al., 2019) as base model to stay consistent with previous work and the be able to use existing code bases to ensure implementational accuracy. For the INAS dataset, we use PubMedBERT-base-uncased (Gu et al., 2021), since it shows strong performance on the standard classification task for this dataset (Brinner et al., 2022). These base classifiers are used for all base-line methods, and for all parts of the pipelines (encoder, predictor, base classifier, etc.).

Input Processing During training, samples that exceed the 510 token limit for BERT models were split into multiple segments, and one segment was chosen randomly for this model update. For the evaluation, we again split each sample into smaller parts that adhere to the token limit and that overlap for 100 tokens. Scores were predicted for each split separately and linearly blended afterwards.

Model Selection During training, evaluations on the validation set were performed after each epoch, and the best-performing version of the model was selected for testing. On the INAS dataset, the agreement of the predicted rationales with the human annotations was evaluated after each epoch, and the mean of all five scores (AUC-PR, Token-F1, D-Token-F1, IoU-F1, D-IoU-F1) was taken as performance indicator. On the movie dataset, this procedure was not possible, since the data distribution of the validation and test samples is different, meaning that validation results are not a good indicator for performance on the test set. Especially the span-level evaluation scores were unsuitable, since much shorter spans were annotated on the validation set. We chose to use the AUC-PR as performance measure, since it still indicates the models ability to generally recognize useful words.

A.3 **RTP Objective Details**

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We use two regularizers in the optimization objective for our rationalized transformer predictor. The first is a sparsity regularizer that ensures that only a subset of tokens is selected as rationale:

$$\Omega_{\lambda} = \sum_{c \in \mathbf{y}} \alpha_1 \cdot \operatorname{mean}(\mathbf{m}^c)^2 + \alpha_2 \cdot \operatorname{mean}(\mathbf{m}^c)$$

$$+ \sum_{c \in \mathbf{y}} \alpha_3 \cdot \operatorname{mean}(\mathbf{m}^c)^2 + \alpha_4 \cdot \operatorname{mean}(\mathbf{m}^c)$$
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In summary, we perform L1 and L2 regularization 1065 on the mask means for the masks of the ground 1066 truth classes and non-ground-truth classes. In our 1067 experiments, we used $\alpha_1 = 0.2$ and $\alpha_3 = 0.05$, 1068 meaning that regularization for masks of incorrect 1069 classes is weaker. We chose this setting, since for 1070 incorrect classes there is no signal that forces words 1071 the be unmasked, so that less strong regularization is required. The L1 parameters are set to rather low 1073 values of $\alpha_2 = \alpha_4 = 0.001$.

The smoothness regularizer has the following form:

$$\Omega_{\sigma} = \beta_1 \cdot \sum_{c \in \mathcal{Y}} \operatorname{mean}((\boldsymbol{\sigma}^c - \beta_2)^2)$$
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Here, the inner subtraction is meant to be elementwise, so that we regularize each individual sigma value towards a value of β_2 . The actual hyperparameters used are $\beta_1 = 0.02$ and $\beta_2 = 3$.

Finally, we use individual weights for each major component of the optimization objective (Equation 8):

$$\underset{M}{\operatorname{arg\,min}} \begin{array}{l} \gamma_{1} \cdot \mathbf{CE}(M(\mathbf{x}), \mathbf{y}) \\ + \sum_{c \in \mathbf{y}} \left[\gamma_{2} \cdot \mathcal{L}^{c} + \gamma_{3} \cdot \mathcal{L}^{\overline{c}} \right] \\ + \gamma_{4} \cdot \Omega_{\lambda} \\ + \gamma_{5} \cdot \Omega_{\sigma} \end{array}$$

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These values are set to $\gamma_1 = 2$, $\gamma_2 = 5$, $\gamma_3 = 10$, 1086 $\gamma_4 = 6$ and $\gamma_5 = 6$. 1087

A.4 Evaluation Post-Processing

In the INAS dataset, rationales do not cross sen-1089 tence boundaries. For that reason, we opted to 1090 employ a post-processing step that uses SciSpacy 1091 (Neumann et al., 2019) to split each abstract into 1092 sentences, and set the rationale score of the last 1093 token in each sentence (that corresponds to punctu-1094 ation) to 0. This is done for all methods and gen-1095 erally lead to a slight improvement in agreement scores. 1097

B Examples

B.1 Movie Reviews Dataset

Figure 2: An exemplary output of the RTP for a positive review from the movie reviews dataset. Green text indicates the ground-truth annotations.

writing a screenplay for a thriller is hard . harder than pouring concrete under the texas sun . harder than building a bridge over troubled waters . and incidentally , a whole heck of a lot harder
thanwriting a movie review. thrillers are all variations on a theme. you have a smart, resourceful, and powerful bad guy, who has a goal he has to meet. you have a noble and brave good guy,
whohas to protect the innocent, kill the bad guy, and not get killed himself in the process. the trick of thriller writing is doing all of this in an interesting and novel manner. this simple
formulacan lead to classic movies like north by northwest, high noon, or silence of the lambs, or big summer blockbusters like men in black, the fugitive, or air force one, or it can lead to
utterdreck like masterminds, event horizon, kull the conqueror is anyone else getting depressed here? point is it is not explain to follow the formula, you've got to throw in
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imigo do , but it is absolutely necessary in every way. Window that something extra - whether it is a great plot of a weil-whitten screenplay, or great special effects of great locations of
great casting of great performances of great big hungry dinosaurs - the movie rais , that is why the jackar, with all its starpower, with all its budget, with all its hype, gets a big fat f.
brucewillis is the bad guy, the jackal, a legendary killer for hire, richard gere is the good guy, a former ira assassin with a vendetta against the jackal, the jackal is trying to kill someone
.gere is trying to stop him . will gere be able to stop the assassination in time and kill the jackal? (i'll give you three guesses, and the first two do n't count.) there are no surprises
awaiting the audience in the jackal, no moment when you say to yourself, " i wonder what happens next ?" the script for the jackal is n't ripped straight from today's headlines. it 's ripped
off, straight from an episode of millennium, throughout the movie, we learn what the jackal's plans are and how he intends to accomplish them, no surprise, the fun of a movie like this should
comefrom richard gere figuring out what the jackal's plan is and developing a clever plan to foil the bad guy, instead, we get two (count'em, two) scenes where gere is sitting in an fbi
conference room somewhere and instantly divines the jackal's plan just as if he's frank black (or more likely, just as if he's been banded a conv of the script) and we never get more than a
competencies and motivative and motivative and the plantation of the provide a state of the second and a state of the second and the state of the second and the state of the second and the second and the state of the second and the
superinciacue as to why gete has had this hash of maight. It is like gete is character is psychic, but return in or the hold the bit (of the screen where s) seen to know it, and just like in
millennium, the bad guy has an overwhelming need to go after the people the good guy cares about, whether or not they are important to what he is trying to do or not, what is more, in the last
halfof the movie, the jackal, supposedly a super - smart professional terrorist who never makes a mistake, comes down with a major case of the stupids. as for the performances bruce willis
managesto get through the whole movie without a wisecrack, which is a major achievement, but not enough reason to see the movie. his disguises are good, but not as good or as interesting as val
kilmer's in the saint, richard gere is made to talk the entire movie in an irish accent, which detracts from his otherwise lifeless and dull performance, sidney politier is probably the most
disappointingelement in a overwhelmingly disappointing movie - not that his performance is bad or anything, it's not, but it is sad that hollywood won't use this talented actor in any part
other than an thi agent (shoot to kill speakers) writing a good plot and a good screenplay, like i said is hard, but it can be done, it was n't done here, it is our job as consumers to
any and and screenplays and to denote the share the and real and the screenplay multiplay the and the trade of the screenplay is the screenplay and the screenplay is the screenplay and the screenplay is the screenplay and the screenplay is the screenplay is the screenplay and the screenplay is the screenplay and the screenplay is the
reventigeout soften pays and to demonte bad and animer canny ones a for the go see this movie, you in only choosing on the to see this movie, you in only choosing on the to see the the section of the section secti
inejackal, or in the line of life, or a life safety video, for crying out loud, anything other than the jackal, which lives up to its hame by ghawing the dead bones of other, better movies.

Figure 3: An exemplary output of the RTP for a negative review from the movie reviews dataset. Green text indicates the ground-truth annotations.

B.2 INAS Dataset

filing in the gaps: modelling interesting the family invasions using spatially incomplete data . detailed knowledge of patterns in the species invasions is often lacking even though this knowledge is essential to conservation efforts . however, we cannot afford to wait for complete information on the distribution and abundance of native and harmful invasive species . using information from counties well surveyed for plants across the usa , we developed models to fill data gaps in poorly surveyed areasby estimating the density (number of species km (-2)) of native and non - native plant species . here, we show that use the second of native and non - native plant species . here, we show that use the second of native and non - native plant species . here, we show that use the second of native and non - native plant species . here, we show that use the second of native and non - native plant species . here, we show that use the second of native and non - native plant species . here, we show that use the second of native and non - native plant species . here, we show that use the second of native and non - native plant species . here, we show that use the second of non - native plant species densities . and is the second area appears to have the greatest ratio of non - native plant species . these large - scale models could also be applied to smaller spatial scales or other taxa to set priorities for conservation and invasion mitigation , prevention , and control efforts .

Figure 4: An exemplary output of the RTP for an abstract by Jarnevich et al. (2006), which is included in the INAS dataset. The rationale was created for the *Biotic Resistance Hypothesis* label, with green spans indicating the ground-truth annotations.

offuence of insects and fungal pathogens or individual and population parameters of cirsium arvense in its native and introduced ranges . introduced weeds are hypothesized to be invasive in their
exoticranges due to celease from natural energies, cirsium arvense (californian , canada , or creeping thistle) is a weed of eurasian origin that was inadvertently introduced to new zealand (nz)
where it is presently one of the worst invasive weeds . we tested the 'enemy release hypothesis' (erh) by establishing here is come were supported by the native (europe) and introduced
(nz) ranges of c. arvense. we followed the development and fate of individually labelled shoots and recorded recruitment of new shoots into the population over two years, neurol even y occurrent
hadminimalimpact on shoot height and relative growth rate in either range . however usatural enemies did have a significant effect on shoot population growth and development in the native range .
supporting the erh in year one exclusion of insect herbiveres increased mean population growth by 2.1-3.6 shoots m (-2), and in year two exclusion of pathogens increased mean population
growthby 2.7-4.1 shoots m (-2), exclusion of case the privaces in the native range also increased the probability of shoots developing from the budding to the reproductive growth stage by 4
.0x in the first year, and 13.4x in the second year; but exclusion of pathogens had no effect on shoot development in either year. in accordance with the erh, exclusion of install individual and
cathogensdid not benefit shoot development or population growth in the introduced range , in either range , we found no evidence for an additive benefit of dual exclusion of insects and pathogens ,
andin no case was there an interaction between insect and pathogen exclusion, this study further demonstrates the value of conducting manipulative experiments in the native and introduced ranges of

Figure 5: An exemplary output of the RTP for an abstract by Cripps et al. (2011), which is included in the INAS dataset. The rationale was created for the *Enemy Release Hypothesis* label, with green spans indicating the ground-truth annotations.

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