Appendix

A Acronyms

Table 3: Acronym Definitions

Acronym	Meaning
pos	positive
neg	negative
IG	Integrated Gradients [47]
IH	Integrated Hessians [25]
MAHE	Model-Agnostic Hierarchical Explanations [51]
SI	Shapley Interaction Index [20]
STI	Shapley Taylor Interaction Index [14]
SCD	Sampling Contextual Decomposition [26]
SOC	Sampling Occlusion [26]
ANOVA	Analysis of Variance [16]
LIME	Locally Interpretable Model-Agnostic Explanations [39]
SHAP	Shapley Additive Explanations [32]
GA2M	Generalized Additive Model with Pairwise Interactions [30]
MS COCO	Microsoft Common Objects in Context [29]
SST	Stanford Sentiment Treebank [44]
BERT	Bidirectional Encoder Representations from Transformers [13]
AUC	Area Under the Receiver Operating Characteristic Curve
COVID	Coronavirus Disease

B Input Dimensionality Reduction

For a black-box model $f : \mathbb{R}^{p'} \to \mathbb{R}$ which takes as input a vector with p' dimensions (e.g. an image, input embedding, etc.) and maps it to a scalar output (e.g. a class logit), we can make `ArchDetect` more efficient by operating on a lower dimensional input encoding $\mathbf{x} \in \mathbb{R}^p$ with p dimensions. To match the dimensionality p' of the input argument of f, we define a transformation function $\xi : \mathbb{R}^p \to \mathbb{R}^{p'}$ which takes the input encoding $\mathbf{x}$ in the lower dimensional space p and brings it back to the input space of f with dimensionality p'. In other words, (4) becomes

$$\omega_{i,j}(\mathbf{x}) = \left(\frac{1}{h_i h_j}\left(f'(\mathbf{x}^\star_{\{i,j\}} + \mathbf{x}_{\setminus\{i,j\}}) - f'(\mathbf{x}'_{\{i\}} + \mathbf{x}^\star_{\{j\}} + \mathbf{x}_{\setminus\{i,j\}}) - f'(\mathbf{x}^\star_{\{i\}} + \mathbf{x}'_{\{j\}} + \mathbf{x}_{\setminus\{i,j\}}) + f'(\mathbf{x}'_{\{i,j\}} + \mathbf{x}_{\setminus\{i,j\}})\right)\right)^2,$$

where $f' = f \circ \xi$. Correspondingly, `ArchAttribute` (2) becomes

$$\phi(\mathcal{I}) = f'(\mathbf{x}^\star_{\mathcal{I}} + \mathbf{x}'_{\setminus\mathcal{I}}) - f'(\mathbf{x}').$$

Examples of input encodings are discussed for the following data types:

- For an image, we use a superpixel segmenter, which selects regions on the image. The selection is covered by the vector $\mathbf{x} \in \{0,1\}^p$, which encodes which image segments have been selected. Note that wherever $\mathbf{x}$ is 0 corresponds to a baseline feature value (e.g. zeroed image pixels).
- For text, we use the natural correspondence between an input embedding and a word token. The selection of input embedding vectors is also covered by the vector $\mathbf{x} \in \{0,1\}^p$.
- For recommendation data, we use the same type of correspondence between an input embedding and a feature field.

Similar notions of input encodings have also been used in [39, 48].

C Completeness Axiom

Lemma 2 (Completeness on $\mathcal{S}$)**.** *The sum of all attributions by* `ArchAttribute` *for the disjoint sets in $\mathcal{S}$ equals the difference of f between $\mathbf{x}^\star$ and the baseline $\mathbf{x}'$: $f(\mathbf{x}^\star) - f(\mathbf{x}')$.*

Proof. Based on the definition of non-additive statistical interaction (Def. 1), a function f can be represented as a generalized additive function [49–51], here on the domain of $\mathcal{X}$:

$$f(\mathbf{x}) = \sum_{i=1}^{\eta} q_i(\mathbf{x}_{\mathcal{I}_i^u}) + \sum_{j=1}^{p} q'_j(x_j) + b, \tag{6}$$

where $q_i(\mathbf{x}_{\mathcal{I}_i^u})$ is a function of each interaction $\mathcal{I}_i^u$ on $\mathcal{X}$ $\forall i = 1, \dots, \eta$ interactions, $q'_j(x_j)$ is a function for each feature $\forall j = 1, \dots, p$, and b is a bias. The u in $\mathcal{I}^u$ stands for "unmerged".

The disjoint sets of $\mathcal{S} = \{\mathcal{I}_i\}_{i=1}^s$ are the result of merging overlapping interaction sets and main effect sets, so we can merge the subfunctions $q(\cdot)$ and $q'(\cdot)$ of (6) whose input sets overlap to write $f(\mathbf{x})$ as a sum of new functions $g_i(\mathbf{x}_{\mathcal{I}_i})$ $\forall i = 1, \dots, s$:

$$f(\mathbf{x}) = \sum_{i=1}^{s} g_i(\mathbf{x}_{\mathcal{I}_i}) + b. \tag{7}$$

For some $\{g_i\}_{i=1}^s$ of the form of (7), we rewrite (2) by separating out the effect of index i:

$$\phi(\mathcal{I}_i) = f(\mathbf{x}^\star_{\mathcal{I}_i} + \mathbf{x}'_{\setminus \mathcal{I}_i}) - f(\mathbf{x}') \quad \forall i = 1, \dots, s$$

$$= \left(g_i(\mathbf{x}^\star_{\mathcal{I}_i}) + \sum_{\substack{j=1 \\ j \neq i}}^{s} g_j(\mathbf{x}'_{\mathcal{I}_j}) + b \right) - \left(g_i(\mathbf{x}'_{\mathcal{I}_i}) + \sum_{\substack{j=1 \\ j \neq i}}^{s} g_j(\mathbf{x}'_{\mathcal{I}_j}) + b \right) \tag{8}$$

$$= g_i(\mathbf{x}^\star_{\mathcal{I}_i}) - g_i(\mathbf{x}'_{\mathcal{I}_i}). \tag{9}$$

Since all $\mathcal{I} \in \mathcal{S}$ are disjoint, $g_j(\mathbf{x}'_{\mathcal{I}_j})$ can be canceled in (8) $\forall j$, leading to (9). The result at (9) can also be obtained with an alternative attribution approach, as shown in Corollary 6.

Next, we compute the sum of attributions:

$$\sum_{i=1}^{s} \phi(\mathcal{I}_i) = \sum_{i=1}^{s} \left(g_i(\mathbf{x}^\star_{\mathcal{I}_i}) - g_i(\mathbf{x}'_{\mathcal{I}_i}) \right) \tag{10}$$

$$= \sum_{i=1}^{s} g_i(\mathbf{x}^\star_{\mathcal{I}_i}) - \sum_{i=1}^{s} g_i(\mathbf{x}'_{\mathcal{I}_i}) \tag{11}$$

$$= f(\mathbf{x}^\star) - f(\mathbf{x}')$$

□

D Completeness of a Complementary Attribution Method

Corollary 6 (Completeness of a Complement)**.** *An attribution approach: $\phi(\mathcal{I}) = f(\mathbf{x}^\star) - f(\mathbf{x}'_{\mathcal{I}} + \mathbf{x}^\star_{\setminus \mathcal{I}})$, similar to what is mentioned in [26, 28], also satisfies the completeness axiom.*

Proof. Based on Eqs. 7 - 9 of Lemma 2:

$$\phi(\mathcal{I}_i) = f(\mathbf{x}^\star) - f(\mathbf{x}'_{\mathcal{I}_i} + \mathbf{x}^\star_{\setminus \mathcal{I}_i})$$

$$= \left(g_i(\mathbf{x}^\star_{\mathcal{I}_i}) + \sum_{\substack{j=1 \\ j \neq i}}^{s} g_j(\mathbf{x}^\star_{\mathcal{I}_j}) + b \right) - \left(g_i(\mathbf{x}'_{\mathcal{I}_i}) + \sum_{\substack{j=1 \\ j \neq i}}^{s} g_j(\mathbf{x}^\star_{\mathcal{I}_j}) + b \right)$$

$$= g_i(\mathbf{x}^\star_{\mathcal{I}_i}) - g_i(\mathbf{x}'_{\mathcal{I}_i})$$

We can then resume with (10) of Lemma 2. □

E Set Attribution Axiom

Axiom 3 (Set Attribution). *If $f : \mathbb{R}^p \rightarrow \mathbb{R}$ is a function in the form of $f(\mathbf{x}) = \sum_{i=1}^{s} \varphi_i(\mathbf{x}_{\mathcal{I}_i})$ where $\{\mathcal{I}_i\}_{i=1}^{s}$ are disjoint and functions $\{\varphi_i(\cdot)\}_{i=1}^{s}$ have roots, then an interaction attribution method admits an attribution for feature set $\mathcal{I}_i$ as $\varphi_i(\mathbf{x}_{\mathcal{I}_i})\ \forall i = 1, \ldots, s$.*

Lemma 4 (Set Attribution on $\mathcal{S}$). *For $\mathbf{x} = \mathbf{x}^\star$ and a baseline $\mathbf{x}'$ such that $\varphi_i(\mathbf{x}'_{\mathcal{I}_i}) = 0\ \forall i = 1, \ldots, s$,* `ArchAttribute` *satisfies the Set Attribution axiom and provides attribution $\varphi_i(\mathbf{x}_{\mathcal{I}_i})$ for set $\mathcal{I}_i\ \forall i$.*

Proof. From (9) in Lemma 2, `ArchAttribute` can be written as

$$\phi(\mathcal{I}_i) = g_i(\mathbf{x}^\star_{\mathcal{I}_i}) - g_i(\mathbf{x}'_{\mathcal{I}_i}) \quad \forall i = 1, \ldots, s,$$

where $f(\mathbf{x}) = \sum_{i=1}^{s} g_i(\mathbf{x}_{\mathcal{I}_i}) + b$. Since $\mathcal{S} = \{\mathcal{I}_i\}_{i=1}^{s}$ are disjoint feature sets for the same function f in Axiom 3, $g_i(\cdot)$ and $\varphi_i(\cdot)$ are related by a constant bias b_i:

$$\varphi_i(\mathbf{x}) = g_i(\mathbf{x}) + b_i$$

Each $\varphi_i(\cdot)$ has roots, so $g_i(\mathbf{x}) + b_i$ has roots. $\mathbf{x}'$ is set such that $\varphi_i(\mathbf{x}'_{\mathcal{I}_i}) = g_i(\mathbf{x}'_{\mathcal{I}_i}) + b_i = 0$. Rearranging,

$$-g_i(\mathbf{x}'_{\mathcal{I}_i}) = b_i.$$

Adding $g_i(\mathbf{x}^\star_{\mathcal{I}_i})$ to both sides,

$$g_i(\mathbf{x}^\star_{\mathcal{I}_i}) - g_i(\mathbf{x}'_{\mathcal{I}_i}) = g_i(\mathbf{x}^\star_{\mathcal{I}_i}) + b_i,$$

which becomes

$$\phi(\mathcal{I}_i) = \varphi_i(\mathbf{x}^\star_{\mathcal{I}_i}) \quad \forall i = 1, \ldots, s.$$

□

E.1 Set Attribution Counterexamples

We now provide counterexamples to identify situations in which the related methods do not satisfy the Set Attribution axiom.

Let

$$f(\mathbf{x}) = \text{ReLU}(x_1 + x_3 + 1) + \text{ReLU}(x_2) + 1.$$

$f(\mathbf{x})$ can be written as $f(\mathbf{x}) = \varphi_1(\mathbf{x}_{\{1,3\}}) + \varphi_2(\mathbf{x}_{\{2\}})$ where $\varphi_1(\mathbf{x}) = \text{ReLU}(x_1 + x_3 + 1)$, and $\varphi_2(\mathbf{x}) = \text{ReLU}(x_2) + 1$. According to the Set Attribution axiom, an interaction attribution method admits attributions as

- $\text{ReLU}(x_1 + x_3 + 1)$ for features $\mathcal{I}_1 = \{1, 3\}$
- $\text{ReLU}(x_2) + 1$ for feature $\mathcal{I}_2 = \{2\}$.

The above setting serves as counterexamples to the related methods as follows:

- CD always assigns $\alpha + \frac{\alpha}{\alpha+\beta}$ to $\mathcal{I}_1$ and $\beta + \frac{\beta}{\alpha+\beta}$ to $\mathcal{I}_2$, where $\alpha = \text{ReLU}(x_1 + x_3 + 1)$ and $\beta = \text{ReLU}(x_2)$.
- SCD uses an expectation over an activation decomposition, which does not guarantee admission of $\text{ReLU}(x_1 + x_3 + 1)$ for $\mathcal{I}_1$ and $\text{ReLU}(x_2)$ for $\mathcal{I}_2$ through their respective decompositions. In the ideal case SCD becomes CD, which still does not satisfy Set Attribution from above.
- IH always assigns a zero attribution to $\mathcal{I}_2$ from hessian computations. IH also does not assign attributions to general sets of features.
- SOC does not assign attributions to general feature sets, only contiguous feature sequences.
- Both SI and STI assign the following attribution score to $\mathcal{I}_1$:

  $$\text{ReLU}(x_1 + x_3 + 1) - \text{ReLU}(x_1 + x'_3 + 1) - \text{ReLU}(x'_1 + x_3 + 1) + \text{ReLU}(x'_1 + x'_3 + 1). \quad (12)$$

  There do not exist a selection of x'_1 and x'_3 such that this attribution becomes $\text{ReLU}(x_1 + x_3 + 1)$ for all values of x_1 and x_3.

Proof. We prove via case-by-case contradiction. Only the $\text{ReLU}(x_1 + x_3 + 1)$ term can create an interaction between x_1 and x_3, and this term is also the target result, so any nonzero deviation from this term via independent x_1 or x_3 effects in (12) must be countered. These independent effects manifest as the $\text{ReLU}(x_1 + x_3' + 1)$ or $\text{ReLU}(x_1' + x_3 + 1)$ terms respectively. Since ReLU is always non-negative, the only way either of these terms is nonzero is if it is positive, which implies that $\text{ReLU}(x_1 + x_3' + 1) = x_1 + x_3' + 1$ or $\text{ReLU}(x_1' + x_3 + 1) = x_1' + x_3 + 1$. If both terms are positive, their substitution into (12) yields $\text{ReLU}(x_1 + x_3 + 1) - x_1 - x_3' - 1 - x_1' - x_3 - 1 + \text{ReLU}(x_1' + x_3' + 1)$. Even if $\text{ReLU}(x_1' + x_3' + 1)$ is positive, we obtain $\text{ReLU}(x_1 + x_3 + 1) - x_1 - x_3' - 1 - x_1' - x_3 - 1 + x_1' + x_3' + 1 = \text{ReLU}(x_1 + x_3 + 1) - x_1 - x_3 - 1$. Asserting $-x_1 - x_3 - 1 = 0$ is a contradiction. If only one of the independent effects was positive, we also cannot assert 0 through similar simplifications.

Now consider the remaining case where $\text{ReLU}(x_1 + x_3' + 1) = \text{ReLU}(x_1' + x_3 + 1) = \text{ReLU}(x_1' + x_3' + 1) = 0$. For any real-valued x_1' or x_3', there can also be a negative real-valued x_3 or x_1 respectively. From either terms $\text{ReLU}(x_1 + x_3' + 1)$ or $\text{ReLU}(x_1' + x_3 + 1)$, we obtain $\text{ReLU}(1) = 0$, which is a contradiction. □

F Other Axioms

F.1 Sensitivity

Lemma 7 (Sensitivity (a))**.** *If $\mathbf{x}^\star$ and $\mathbf{x}'$ only differ at features indexed in $\mathcal{I}$ and $f(\mathbf{x}^\star) \neq f(\mathbf{x}')$, then $\phi(\mathcal{I})$ (2) yields a nonzero attribution.*

Proof. Since $\mathbf{x}^\star$ and $\mathbf{x}'$ only differ at $\mathcal{I}$, the following is true: $\mathbf{x}^\star_{\setminus\mathcal{I}} = \mathbf{x}'_{\setminus\mathcal{I}}$. We can therefore write $\mathbf{x}^\star$ as

$$\begin{aligned}\mathbf{x}^\star &= \mathbf{x}^\star_{\mathcal{I}} + \mathbf{x}^\star_{\setminus\mathcal{I}}\\ &= \mathbf{x}^\star_{\mathcal{I}} + \mathbf{x}'_{\setminus\mathcal{I}}\end{aligned}$$

Substituting this equivalence in (2), we have

$$\begin{aligned}\phi(\mathcal{I}) &= f(\mathbf{x}^\star_{\mathcal{I}} + \mathbf{x}'_{\setminus\mathcal{I}}) - f(\mathbf{x}')\\ &= f(\mathbf{x}^\star) - f(\mathbf{x}').\end{aligned}$$

Since $f(\mathbf{x}^\star) - f(\mathbf{x}') \neq 0$, we directly obtain $\phi(\mathcal{I}) \neq 0$.

□

Lemma 8 (Sensitivity (b))**.** *If f does not functionally depend on $\mathcal{I}$, then $\phi(\mathcal{I})$ is always zero.*

Proof. Since f does not functionally depend on $\mathcal{I}$,

$$\begin{aligned}f(\mathbf{x}^\star_{\mathcal{I}} + \mathbf{x}'_{\setminus\mathcal{I}}) &= f(\mathbf{x}'_{\mathcal{I}} + \mathbf{x}'_{\setminus\mathcal{I}})\\ &= f(\mathbf{x}')\end{aligned}$$

Therefore,

$$\phi(\mathcal{I}) = f(\mathbf{x}^\star_{\mathcal{I}} + \mathbf{x}'_{\setminus\mathcal{I}}) - f(\mathbf{x}') = 0.$$

□

F.2 Implementation Invariance

Lemma 9 (Implementation Invariance)**.** *For functionally equivalent models (with the same input-output mapping), $\phi(\cdot)$ are the same.*

The definition of (2) only relies on function calls to f, which implies Implementation Invariance.

F.3 Linearity

Lemma 10 (Linearity on $\mathcal{S}$)**.** *If two models f_1, f_2 have the same disjoint feature sets $\mathcal{S}$ and $f = c_1 f_1 + c_2 f_2$ where c_1, c_2 are constants, then $\phi(\mathcal{I}) = c_1\phi_1(\mathcal{I}) + c_2\phi_2(\mathcal{I})\ \forall \mathcal{I} \in \mathcal{S}$.*

Proof. Since f_1 and f_2 have the same $\mathcal{S} = \{\mathcal{I}_i\}_{i=1}^{s}$, we can write f_1 and f_2 as follows via (7) in Lemma 2:

$$f_1(\mathbf{x}) = \sum_{i=1}^{s} g_i^{(1)}(\mathbf{x}_{\mathcal{I}_i}) + b^{(1)},$$

$$f_2(\mathbf{x}) = \sum_{i=1}^{s} g_i^{(2)}(\mathbf{x}_{\mathcal{I}_i}) + b^{(2)}.$$

Since $f = c_1 f_1 + c_2 f_2$,

$$\begin{aligned} f(\mathbf{x}) &= c_1 f_1(\mathbf{x}) + c_2 f_2(\mathbf{x}) \\ &= \left(\sum_{i=1}^{s} c_1 \times g_i^{(1)}(\mathbf{x}_{\mathcal{I}_i}) + c_1 \times b^{(1)}\right) + \left(\sum_{i=1}^{s} c_2 \times g_i^{(2)}(\mathbf{x}_{\mathcal{I}_i}) + c_2 \times b^{(2)}\right) \\ &= \sum_{i=1}^{s} \left(c_1 \times g_i^{(1)}(\mathbf{x}_{\mathcal{I}_i}) + c_2 \times g_i^{(2)}(\mathbf{x}_{\mathcal{I}_i})\right) + c_1 b^{(1)} + c_2 b^{(2)}. \end{aligned} \tag{13}$$

By grouping terms as $g_i(\mathbf{x}_{\mathcal{I}_i}) = c_1 \times g_i^{(1)}(\mathbf{x}_{\mathcal{I}_i}) + c_2 \times g_i^{(2)}(\mathbf{x}_{\mathcal{I}_i})$ and $b = c_1 b^{(1)} + c_2 b^{(2)}$, we write (13) as

$$f(\mathbf{x}) = \sum_{i=1}^{s} g_i(\mathbf{x}_{\mathcal{I}_i}) + b. \tag{14}$$

From the form of (14), we can invoke (9): $\phi(\mathcal{I}_i) = g_i(\mathbf{x}^{\star}_{\mathcal{I}_i}) - g_i(\mathbf{x}'_{\mathcal{I}_i})$ via Lemma 2. This equation is rewritten as

$$\begin{aligned} \phi(\mathcal{I}_i) &= g_i(\mathbf{x}^{\star}_{\mathcal{I}_i}) - g_i(\mathbf{x}'_{\mathcal{I}_i}) \\ &= \left(c_1 \times g_i^{(1)}(\mathbf{x}^{\star}_{\mathcal{I}_i}) + c_2 \times g_i^{(2)}(\mathbf{x}^{\star}_{\mathcal{I}_i})\right) - \left(c_1 \times g_i^{(1)}(\mathbf{x}'_{\mathcal{I}_i}) + c_2 \times g_i^{(2)}(\mathbf{x}'_{\mathcal{I}_i})\right) \\ &= c_1 \left(g_i^{(1)}(\mathbf{x}^{\star}_{\mathcal{I}_i}) - g_i^{(1)}(\mathbf{x}'_{\mathcal{I}_i})\right) + c_2 \left(g_i^{(2)}(\mathbf{x}^{\star}_{\mathcal{I}_i}) - g_i^{(2)}(\mathbf{x}'_{\mathcal{I}_i})\right) \\ &= c_1\phi_1(\mathcal{I}_i) + c_2\phi_2(\mathcal{I}_i). \end{aligned}$$

By noting that $\mathcal{S} = \{\mathcal{I}_i\}_{i=1}^{s}$, this concludes the proof.

□

F.4 Symmetry-Preserving

We first define *symmetric feature sets* as a generalization of "symmetric variables" from [47]. Feature index sets $\mathcal{I}_1$ and $\mathcal{I}_2$ are symmetric with respect to function f if swapping features in $\mathcal{I}_1$ with the features in $\mathcal{I}_2$ does not change the function, This implies that for symmetric $\mathcal{I}_1$ and $\mathcal{I}_2$, their cardinalities are the same $|\mathcal{I}_1| = |\mathcal{I}_2|$, and they are disjoint sets in order to swap the features to any valid set index.

Lemma 11 (Symmetry-Preserving)**.** *For $\mathbf{x}^{\star}$ and $\mathbf{x}'$ that each have identical feature values between symmetric feature sets with respect to f, the symmetric feature sets receive identical attributions $\phi(\cdot)$.*

Proof. Since $\mathbf{x}^{\star}$ and $\mathbf{x}'$ each have identical feature values between the symmetric feature sets,

$$\{x_i^{\star}\}_{i \in \mathcal{I}_1} = \{x_j^{\star}\}_{j \in \mathcal{I}_2},$$

$$\{x_i'\}_{i \in \mathcal{I}_1} = \{x_j'\}_{j \in \mathcal{I}_2}.$$

Therefore, the symmetry implies the following for any $\mathbf{x}$ in the domain of f.

$$f\left(\mathbf{x}^{\star}_{\mathcal{I}_1} + \mathbf{x}'_{\mathcal{I}_2} + \mathbf{x}_{\setminus(\mathcal{I}_1\cup\mathcal{I}_2)}\right) = f\left(\mathbf{x}'_{\mathcal{I}_1} + \mathbf{x}^{\star}_{\mathcal{I}_2} + \mathbf{x}_{\setminus(\mathcal{I}_1\cup\mathcal{I}_2)}\right) \tag{15}$$

Setting $\mathbf{x} = \mathbf{x}'$, we rewrite (15) as

$$\begin{aligned}
&f\left(\mathbf{x}^{\star}_{\mathcal{I}_1} + \mathbf{x}'_{\mathcal{I}_2} + \mathbf{x}'_{\setminus(\mathcal{I}_1\cup\mathcal{I}_2)}\right) - f\left(\mathbf{x}'_{\mathcal{I}_1} + \mathbf{x}^{\star}_{\mathcal{I}_2} + \mathbf{x}'_{\setminus(\mathcal{I}_1\cup\mathcal{I}_2)}\right) = 0\\
&= f(\mathbf{x}^{\star}_{\mathcal{I}_1} + \mathbf{x}'_{\setminus\mathcal{I}_1}) - f(\mathbf{x}^{\star}_{\mathcal{I}_2} + \mathbf{x}'_{\setminus\mathcal{I}_2})\\
&= \left(f(\mathbf{x}^{\star}_{\mathcal{I}_1} + \mathbf{x}'_{\setminus\mathcal{I}_1}) - f(\mathbf{x}')\right) - \left(f(\mathbf{x}^{\star}_{\mathcal{I}_2} + \mathbf{x}'_{\setminus\mathcal{I}_2}) - f(\mathbf{x}')\right)\\
&= \phi(\mathcal{I}_1) - \phi(\mathcal{I}_2)
\end{aligned}$$

Therefore, $\phi(\mathcal{I}_1) = \phi(\mathcal{I}_2)$.

□

G Discrete Mixed Partial Derivatives Detect Non-Additive Statistical Interactions

A generalized additive model f_g is given by

$$f_g(\mathbf{x}) = \sum_{i=1}^{p} g_i(x_i) + b, \tag{16}$$

where $g_i(\cdot)$ can be any function of individual features x_i and b is a bias. Since each x_i of $\mathbf{x} \in \mathcal{X}$ only takes on two values, a line can connect all valid points in each feature. Therefore, (16) is equivalent to

$$f_\ell(\mathbf{x}) = \sum_{i=1}^{p} w_i x_i + b, \tag{17}$$

for weights $w_i \in \mathbb{R}$ and the function domain being $\mathcal{X}$.

For the case where $p = 2$, the discrete mixed partial derivative is given by (3) or

$$\frac{\partial^2 f}{\partial x_1 \partial x_2} = \frac{1}{h_1 h_2}\left(f([x_1^\star, x_2^\star]) - f([x_1^\star, x_2']) - f([x_1', x_2^\star]) + f([x_1', x_2'])\right),$$

where $h_1 = |x_1^\star - x_1'|$ and $h_2 = |x_2^\star - x_2'|$. Since any three points (not on the same line) define a plane of the form (17) ($p = 2$), we can write the fourth point as having a function value with deviation δ from the plane.

$$\begin{aligned}
\frac{\partial^2 f}{\partial x_1 \partial x_2} &= \frac{1}{h_1 h_2}\left(f([x_1^\star, x_2^\star]) - f([x_1^\star, x_2']) - f([x_1', x_2^\star]) + f([x_1', x_2'])\right)\\
&= \frac{1}{h_1 h_2}\left((w_1 x_1^\star + w_2 x_2^\star + b + \delta) - (w_1 x_1^\star + w_2 x_2' + b) - (w_1 x_1' + w_2 x_2^\star + b)\right.\\
&\qquad\qquad \left. + (w_1 x_1' + w_2 x_2' + b)\right)\\
&= \frac{\delta}{h_1 h_2}.
\end{aligned} \tag{18}$$

If (18) is 0, then $\delta = 0$, which implies that f can be written as (17). $\delta \neq 0$ implies the opposite, that f cannot be written in linear form (by definition). Since (17) is equivalent to (16) in the domain of $\mathcal{X}$, this implies that $\delta \neq 0$ if and only if $f(\mathbf{x}) \neq g_1(x_1) + g_2(x_2) + b$.

Based on Def. 1, we can conclude that a nonzero discrete mixed partial derivative w.r.t. x_1 and x_2 in the space $\mathcal{X}$ at $p = 2$ detects a non-additive statistical interaction between the two features.

For the case where $p > 2$, Def. 1 states that a pairwise interaction $\{i, j\}$ exists in f if and only if $f(\mathbf{x}) \neq f_i(\mathbf{x}_{\setminus\{i\}}) + f_j(\mathbf{x}_{\setminus\{j\}})$ for functions $f_i(\cdot)$ and $f_j(\cdot)$. This means that $\{i, j\}$ is declared to be an interaction if a local $\{i, j\}$ interaction occurs at any $\mathbf{x}_{\setminus\{i,j\}}$, $\mathbf{x} \in \mathcal{X}$.

Therefore, we can detect non-additive statistical interactions $\{i, j\}$ for general $p \geq 2$ via

$$\mathbb{E}_{\mathbf{x}}\left[\frac{\partial^2 f}{\partial x_i \partial x_j}\right]^2 > 0,$$

which mirrors the definition of pairwise interaction for real-valued $\mathbf{x}$ in [18].

H Early Works on Feature Interaction Interpretation

We discuss early works on feature interaction interpretation and provide a timeline for this research history in Table 4. We also discuss mixed partial derivatives on dichotomous variables in H.3.

H.1 Origins

The notion of a feature interaction has been studied at least since the 19th century when John Lawes and Joseph Gilbert used factorial designs in agricultural research at the Rothamsted Experimental Station [11]. A factorial design is an experiment that includes observations at all combinations of categories of each factor or feature. However, the "advantages [of factorial design] had never been clearly recognised, and many research workers believed that the best course was the conceptually simple one of investigating one question at a time" [58]. In the early 20th century, Fisher et al. (1926) [17] emphasized the importance of factorial designs as being the only way to obtain information about feature interactions. Near the same time, Fisher (1921) [15] also developed one of the foundations of statistical analysis called Analysis of Variance (ANOVA) including two-way ANOVA [16], which is a factorial method to detect pairwise feature interactions based on differences among group means in a dataset. Tukey (1949) [52] extended two-way ANOVA to test if two categorical features are non-additively related to the expected value of a outcome variable. This work set a precedent for later research on detecting feature interactions based on their non-additive definition. Soon after, experimental designs were generalized to study feature interactions, in particular the generalized randomized block design [55], which assigns test subjects to different categories (or blocks) between features in a way where cross-categories between features serve as interaction terms in linear regression.

There was a surge of interest in improving the analysis of feature interactions after the mid 20th century. Belsion (1959) [5] and Morgan & Sonquist (1963) [35] proposed Automatic Interaction Detection (AID) originally under a different name. AID detects interactions by subdividing data into disjoint exhaustive subsets to model an outcome based on categorical features. Based on AID, Kass (1980) [27] developed Chi-square Automatic Interaction Detection (CHAID), which determines how categorical features best combine in decision trees via a chi-square test. AID and CHAID were precursors to modern decision tree prediction models. Concurrently, Nelder (1977) [37] introduced the "Principle of Marginality" arguing that a feature interaction and its marginal variables should not be considered separately, for example in linear regression. Hamada & Wu (1992) [22] provided a contrasting view that an interaction is only important if one or both of its marginal variables are important. Around the same time, an influential book on interpreting feature interactions was published on how to test, plot, and understand interactions of two or three continuous or categorical features [3].

H.2 Early 21st Century Works

At the start of the 21st century, efforts began to focus on interpreting interactions in accurate prediction models. Ai & Norton (2003) [2] proposed extracting interactions from logit and probit models via mixed partial derivatives. Gevrey (2006) [19] followed up by proposing mixed partial derivatives to extract interactions from multilayer perceptrons with sigmoid activations when at the time, only shallow neural networks were studied. Friedman & Popescu (2008) [18] proposed using hybrid models to capture interactions with decision trees and univariate effects with linear regression. Sorokina et al. (2008) [46] proposed to use high-performance additive trees to detect feature interactions based on their non-additive definition. At the turn of the decade, we saw Bien et al. [6] capture interactions with different heredity conditions using a hierarchical lasso on linear regression models. Then, Hao & Zhang (2014) [23] drew attention towards interaction screening in high dimensional data. This summarizes feature interaction research before 2015.

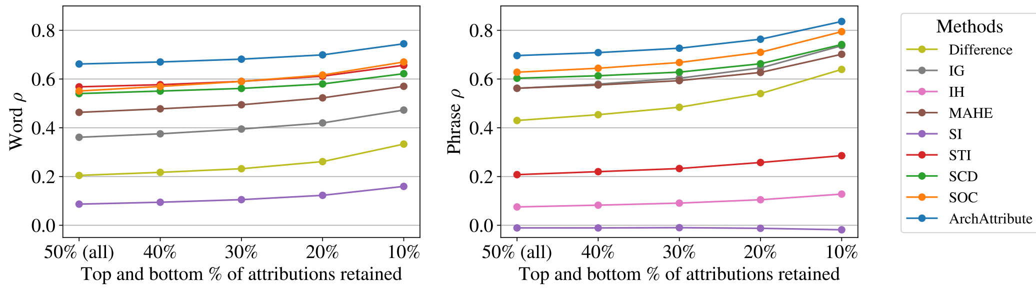
H.3 Note on Mixed Partial Derivatives on Dichotomous Variables

To our knowledge, the usage of mixed partial derivatives for interaction detection on dichotomous variables (features that only take two possible values) originated at the turn of the 21st century [2, 20], but existing methods rely on single contexts [2] or random contexts [14, 20]. Furthermore, these methods do not consider the union of overlapping pairwise interactions for disjoint higher-order interaction detection. Our choice of contexts and our disjoint interaction detection are both important to the `Archipelago` framework, as we discussed in §4.2 and showed through axiomatic analysis (§3.2) and experiments (§5.2).

TABLE 4 Timeline of research on feature interaction interpretation (Pre-2015)

Lawes & Gilbert - factorial design in agricultural research at the Rothamsted Experimental Station	1843	
Fisher - two-way Analysis of Variance (ANOVA)	1925	
	1949	*Tukey* - Tukey's test of additivity
	1955	*Wilk* - generalized random block design
Belson - Automatic Interaction Detection by subdividing data	1959	
Nelder - Principle of Marginality	1977	
	1980	*Kass* - Chi-square Automatic Interaction Detection by combining features in decision trees via chi-square tests
	1991	*Aiken & West* - book on interpreting interaction effects
Hamada & Wu - heredity conditions	1992	
Ai & Norton - interactions in logit and probit models	2003	
	2006	*Gevry et al.* - interactions in sigmoid neural networks
Friedman & Popescu - RuleFit to detect interactions by mixing linear regression and trees	2008	*Sorokina et al.* - Additive Groves to detect non-additive interactions
Bien et al. - Hierarchical Lasso	2013	
Hao & Zhang - interaction screening in high dimensional data	2014	

I Attributions Compared to Annotation Labels



(a) Word ρ (b) Phrase ρ

Figure 9: Text explanation metrics ((a) Word ρ and (b) Phrase ρ) versus top and bottom % of attributions retained for different attribution methods on BERT over the SST test set. These plots expand the analysis of Table 2.

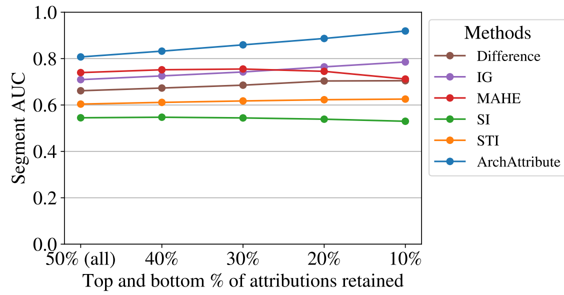


Figure 10: Image explanation metric (segment AUC) versus top and bottom % of attributions retained for different attribution methods on ResNet152 over the MS COCO test set. These plots expand the analysis of Table 2.

J Visualization Comparisons

J.1 Sentiment Analysis

Visualization comparisons of different attribution methods on BERT are shown in Figs. 12-16 for random test sentences from SST. The visualization format is the same as Fig. 4. Note that all *individual* feature attributions that correspond to stop words (from [33]) are omitted in these comparisons and Figs. 1, 4.

J.2 Image Classification

In Fig. 11, we visualize `Archipelago` explanations on $\mathcal{S}$ via top-5 pairwise interactions (§4.2.2), where positive attribution interactions are shown for clarity. The images are randomly selected from the ImageNet test set. It is interesting to see which image parts interact, such as the eyes of the "great dane" image.

Visualization comparisons of different attribution methods on ResNet152 are shown in Figs. 17-21 for the same random test images from ImageNet.

K `ArchDetect` Ablation Visualizations

We run an ablation study removing the $\mathbf{x}'_{\setminus\{i,j\}}$ baseline context from (5) for disjoint interaction detection and examine its effect on visualizations. The visualizations are shown in Fig. 22 for

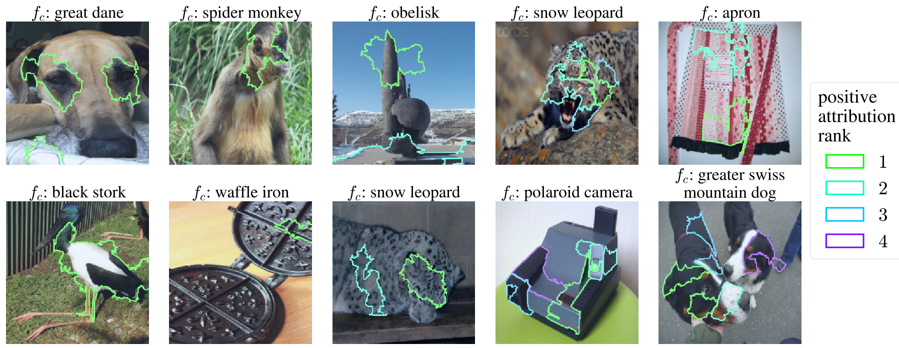


Figure 11: Our ResNet152 visualizations on random test images from ImageNet. Colored outlines indicate interactions with positive attribution. f_c is the image classification result. To our knowledge, only this work shows interactions that support the image classification via interaction attribution.

sentiment analysis and Figs. 23 and 24 for image classification. Top-3 and top-5 pairwise interactions are used in sentiment analysis and image classification respectively before merging the interactions.

L `ArchAttribute` with Different Interaction Detectors

We compare visualizations of `ArchAttribute` using different interaction detectors. The visualizations are shown in Figs. 25 and 26 for sentiment analysis and Figs. 27, 28, and 29 for image classification. Top-3 and top-5 pairwise interactions are used in sentiment analysis and image classification respectively before merging the interactions.

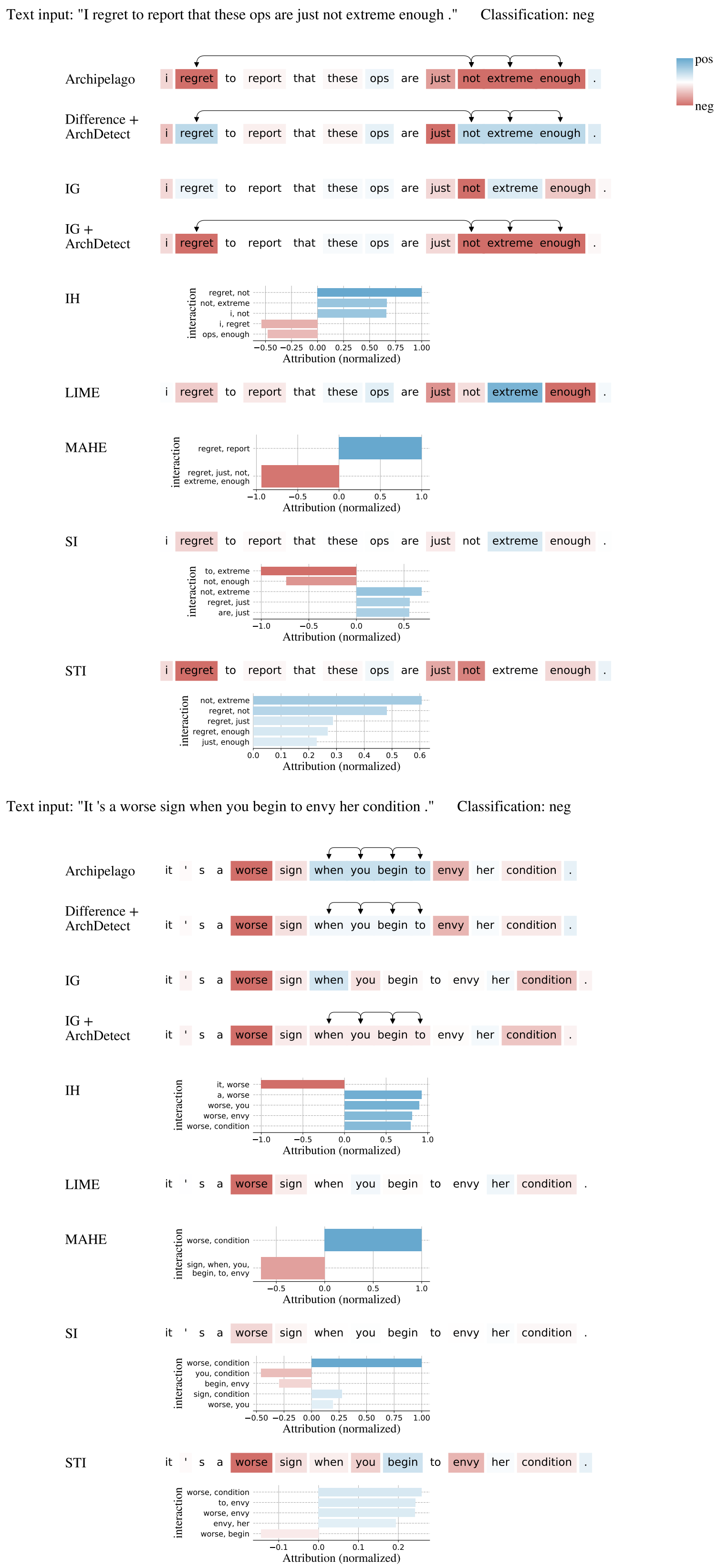


Figure 12: Text Viz. Comparison A. In the first text example, “regret, not extreme enough” is a meaningful and strongly negative interaction. In the second example, “when you begin to” interacts to diminish its overall attribution magnitude.

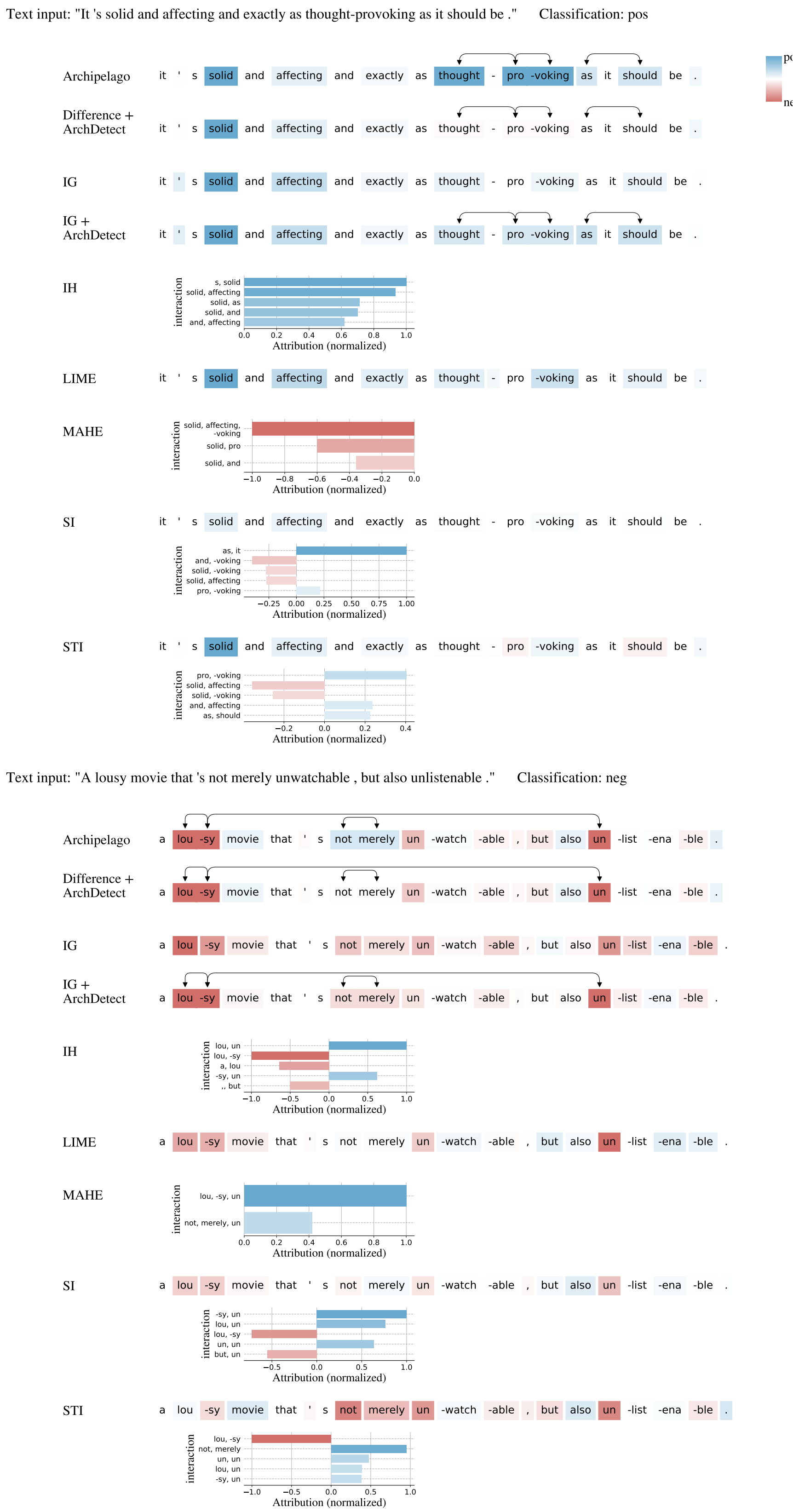


Figure 13: Text Viz. Comparison B. In the first text example, "thought provoking" is a meaningful and strongly positive interaction. In the second example, the "lousy, un" interaction factors in a large context to make a negative text classification.

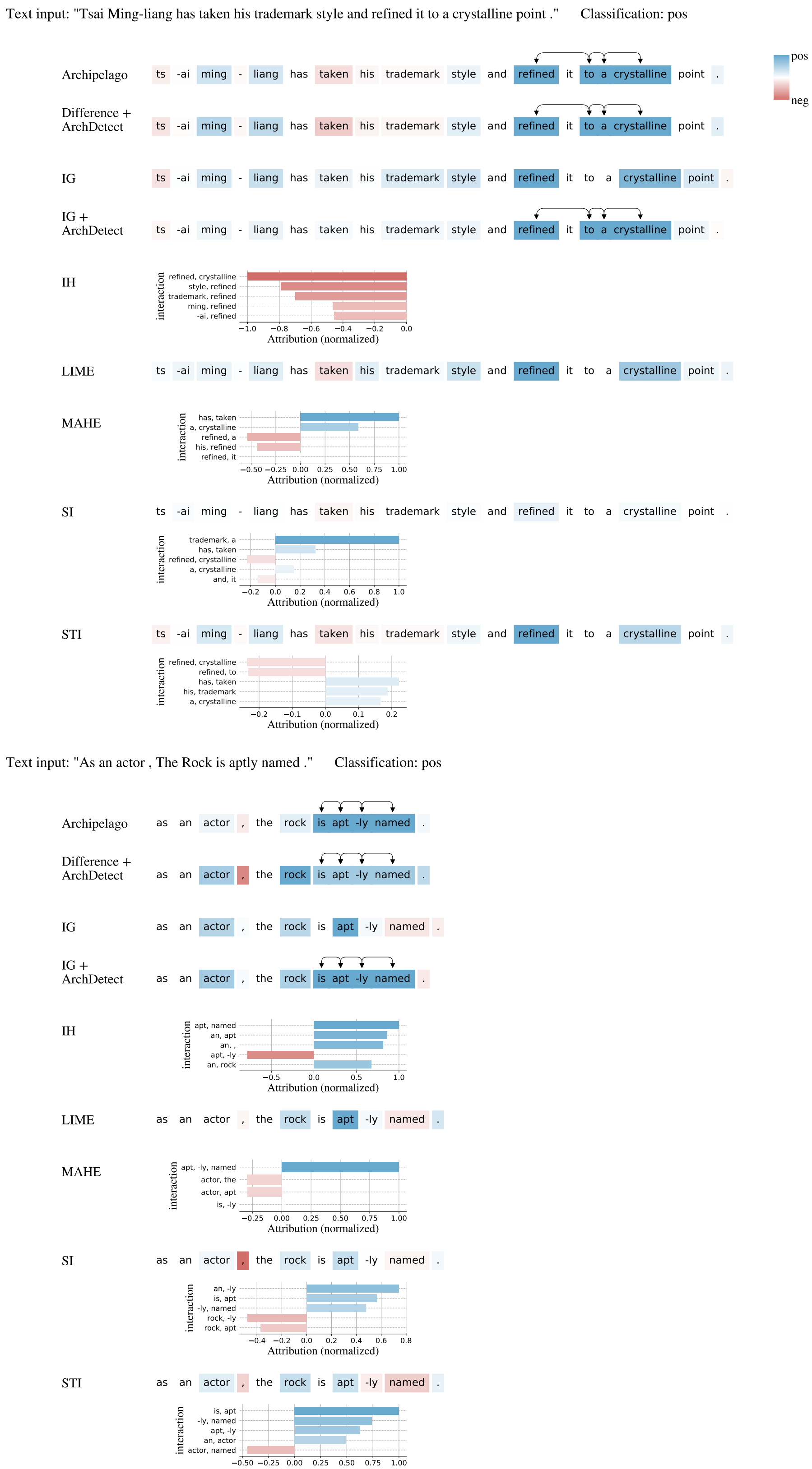


Figure 14: Text Viz. Comparison C. In the first text example, "refined, to a crystalline" is a meaningful and strongly positive interaction. In the second example, "is aptly named" is also a meaningful and strongly positive interaction.

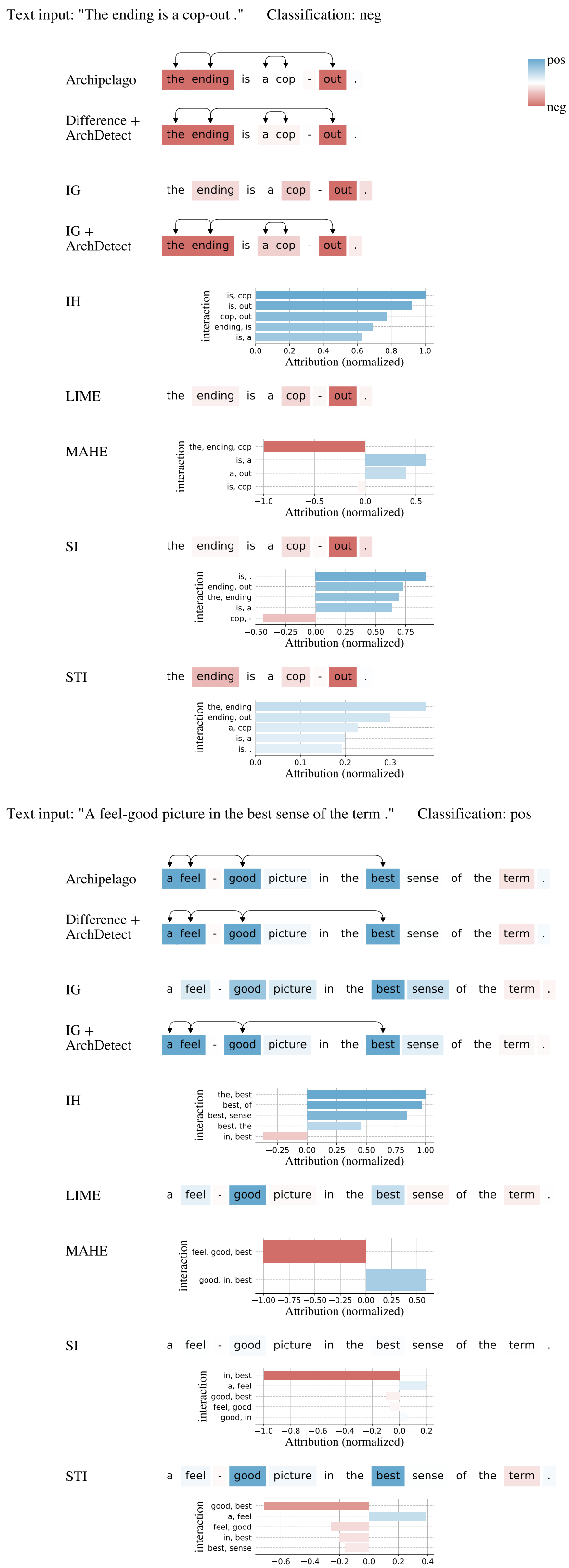


Figure 15: Text Viz. Comparison D. In the first text example, "the ending, out" is a meaningful and negative interaction. In the second example, "a feel good, best" is a meaningful and strongly positive interaction.

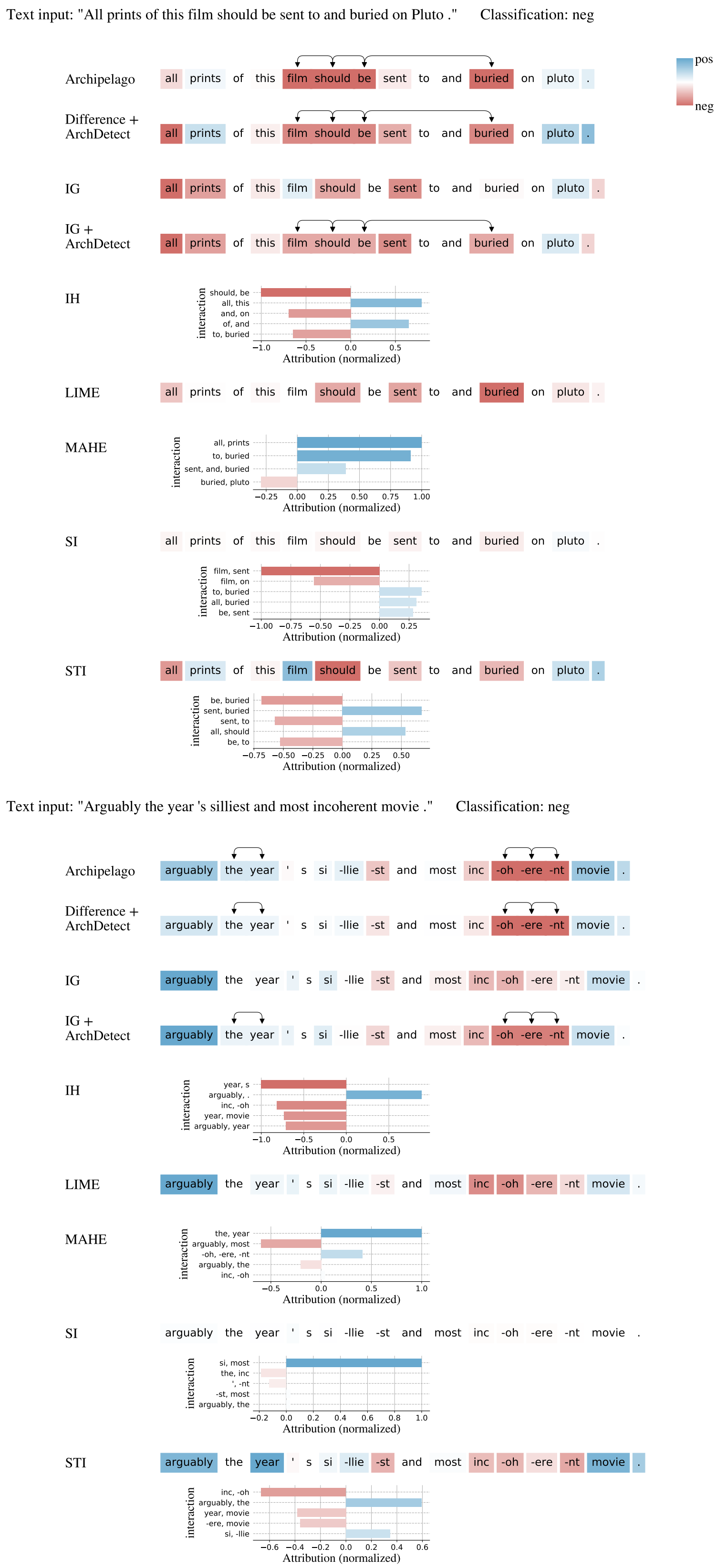


Figure 16: Text Viz. Comparison E. In the first text example, "film should be, buried" is a meaningful and strongly negative interaction. In the second example, "-oherent" belongs to a negative word "incohorent".

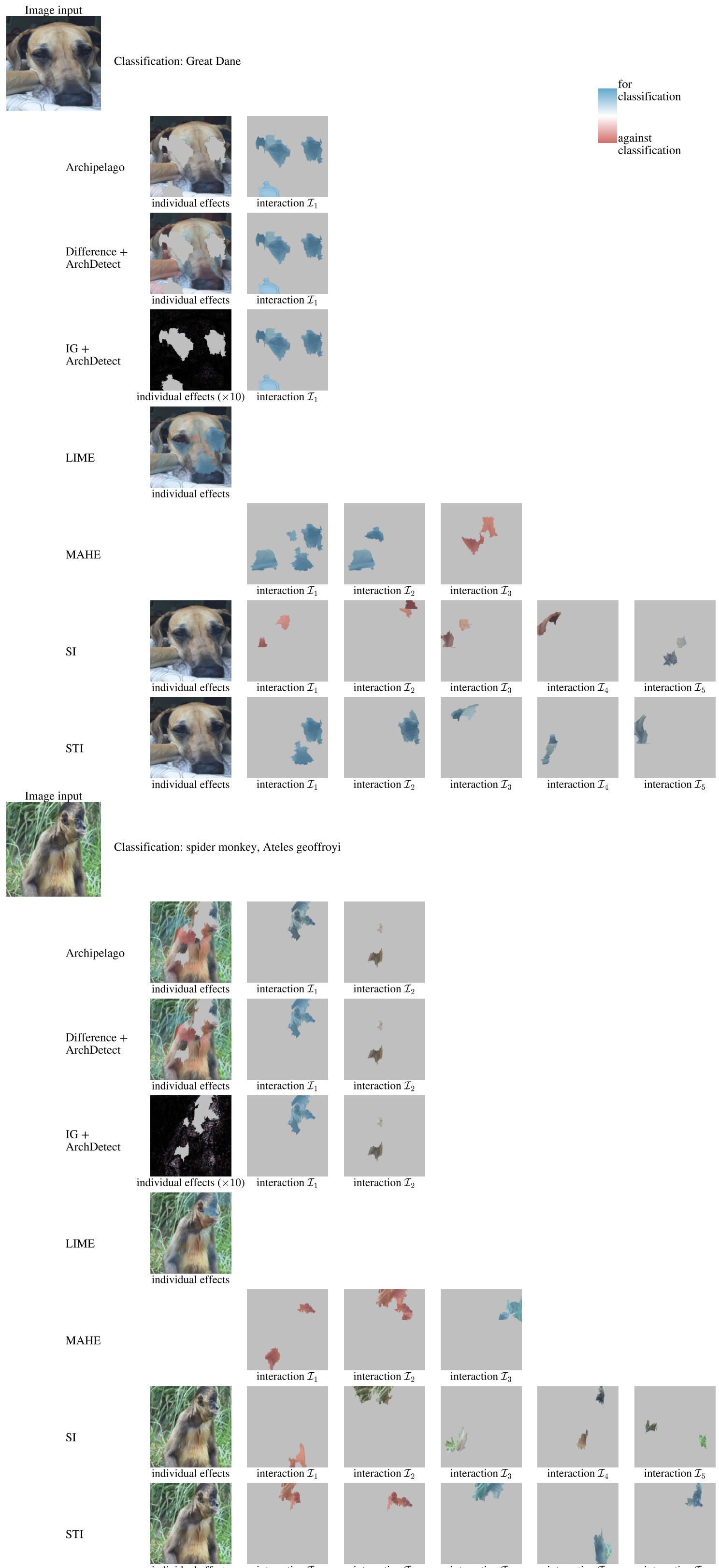


Figure 17: Image Viz. Comparison A. In the first image example, the dog's eyes are a meaningful interaction supporting the classification. In the second example, the monkey's head is also a positive interaction.

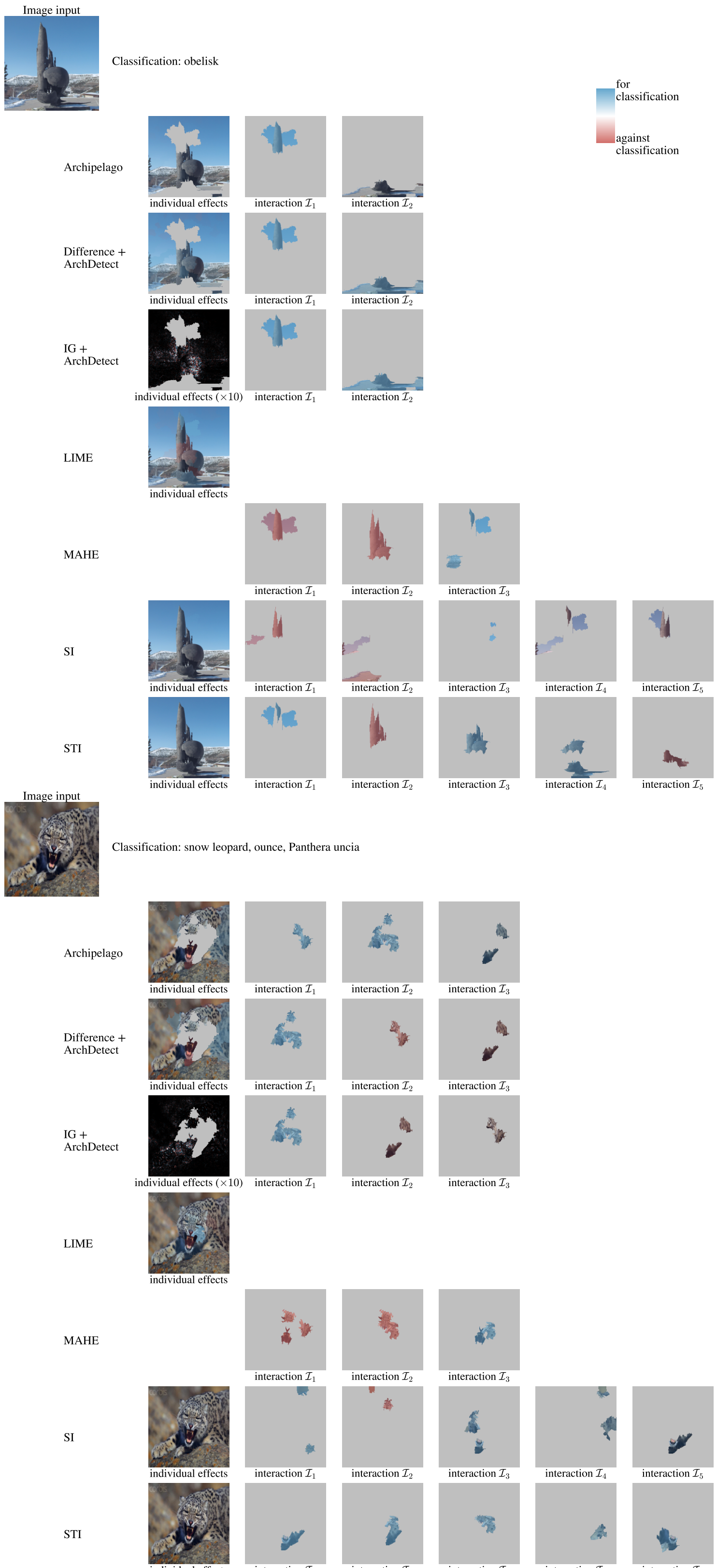


Figure 18: Image Viz. Comparison B. In the first image example, the obelisk tip is a meaningful interaction supporting the classification. In the second example, the leopard's face is also a positive interaction.

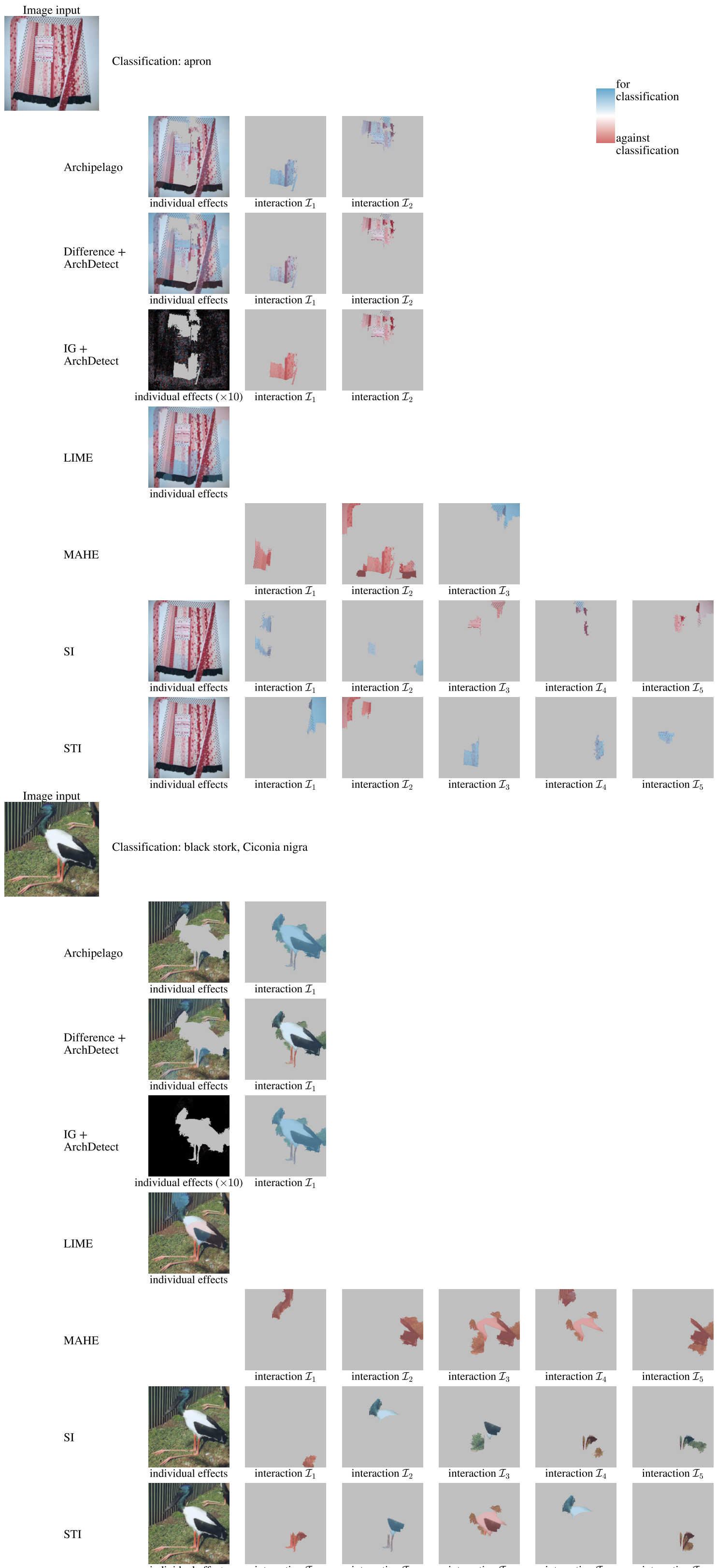


Figure 19: Image Viz. Comparison C. In the first image example, different patches of the apron are interactions supporting the classification. In the second example, the stork's body is an interaction that strongly supports the classification.

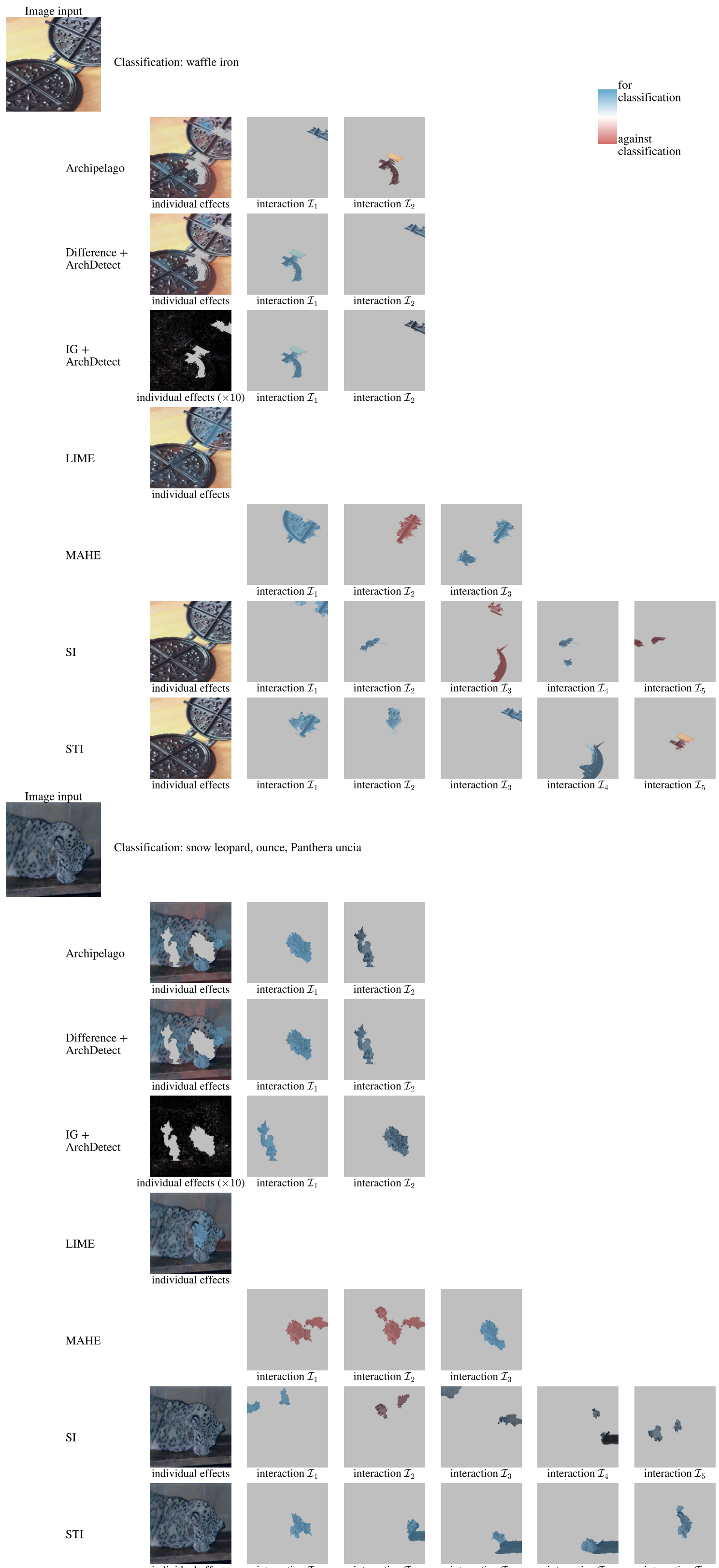


Figure 20: Image Viz. Comparison D. In the first image example, certain small patches of the waffle iron interact, one of which supports the classification. In the second example, the leopard's face is the primary positive interaction.

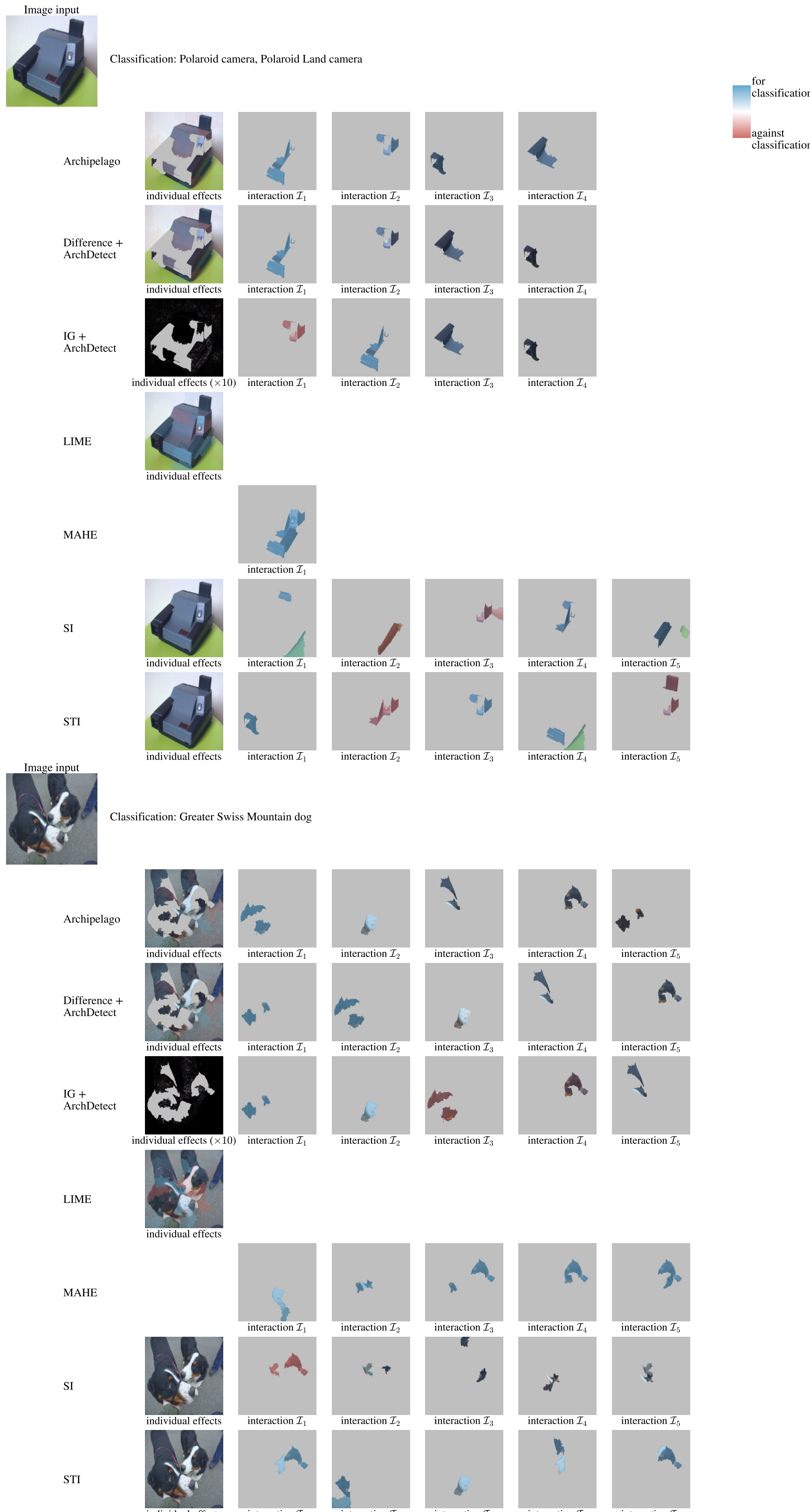


Figure 21: Image Viz. Comparison E. In the first image example, different parts of the polaroid camera are interactions that positively support the classification. In the second example, the dogs' heads and body are also positive interactions.

Figure 22: Text Viz. with `ArchDetect` Ablation. The interactions tend to use more salient words when including the baseline context, which is proposed in `ArchDetect`.

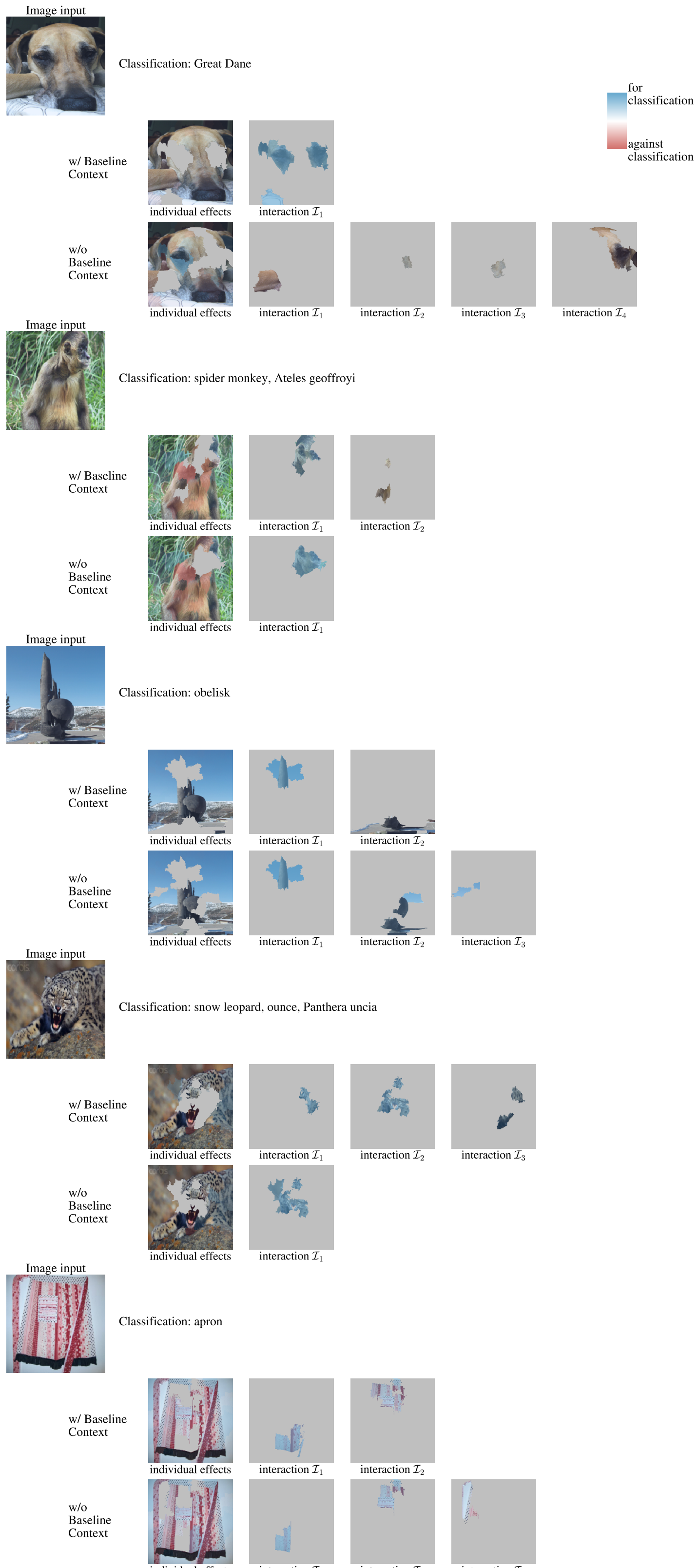


Figure 23: Image Viz. with `ArchDetect` Ablation A. The interactions tend to focus more on salient patches of the images when including the baseline context, which is proposed in `ArchDetect`.

Figure 24: Image Viz. with `ArchDetect` Ablation B. The interactions tend to focus on salient patches of the images when including the baseline context.

Figure 25: Text Viz. with `ArchAttribute` + Different Interaction Detectors A.

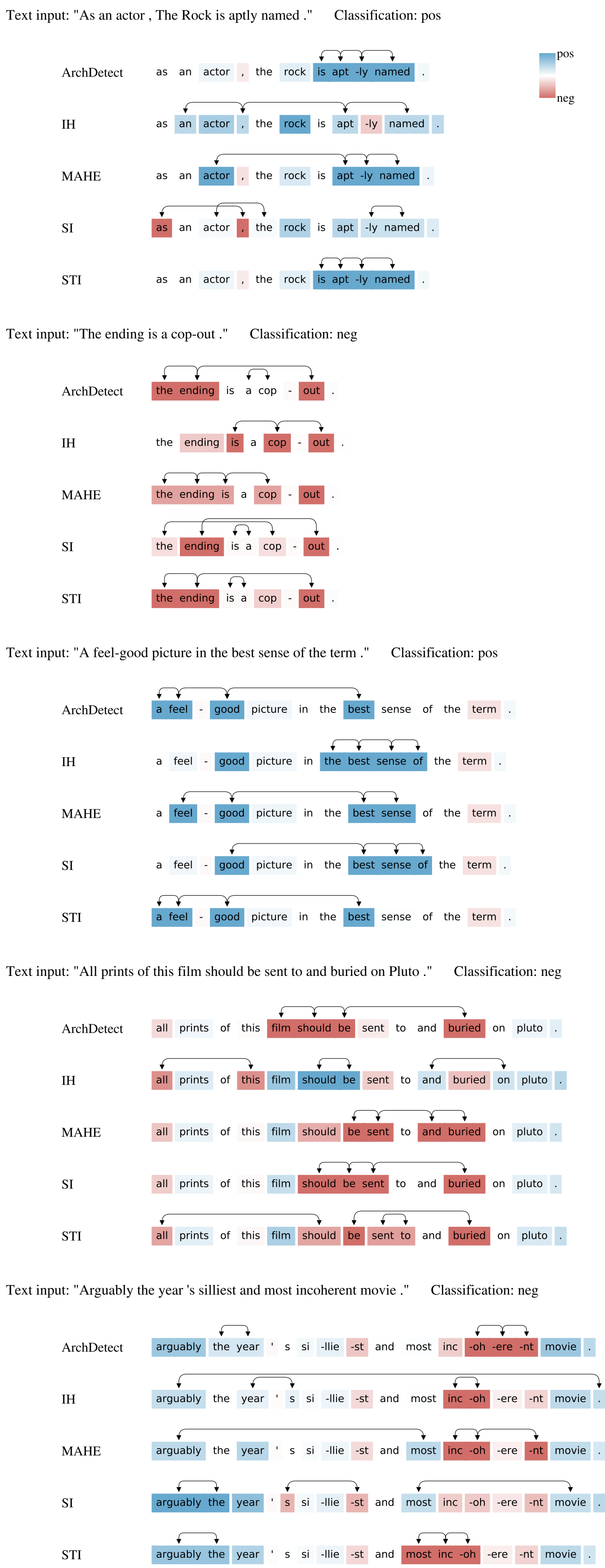


Figure 26: Text Viz. with `ArchAttribute` + Different Interaction Detectors B.

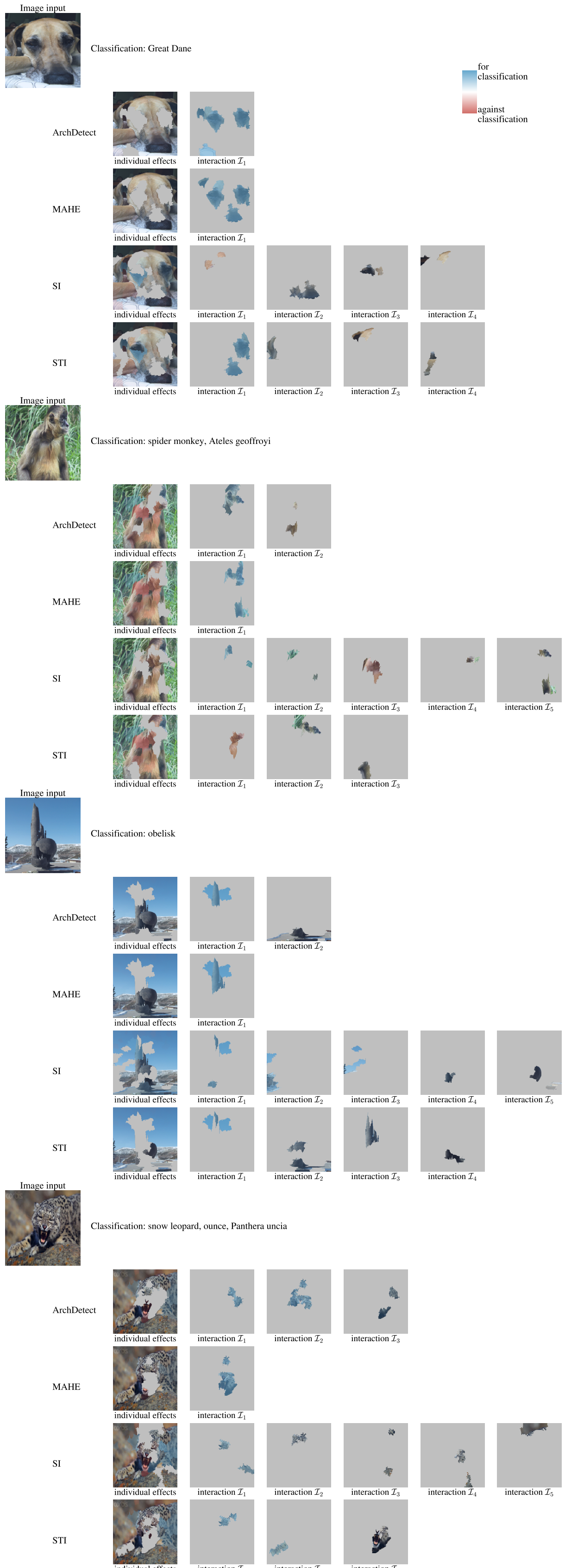


Figure 27: Image Viz. with `ArchAttribute` + Different Interaction Detectors A.

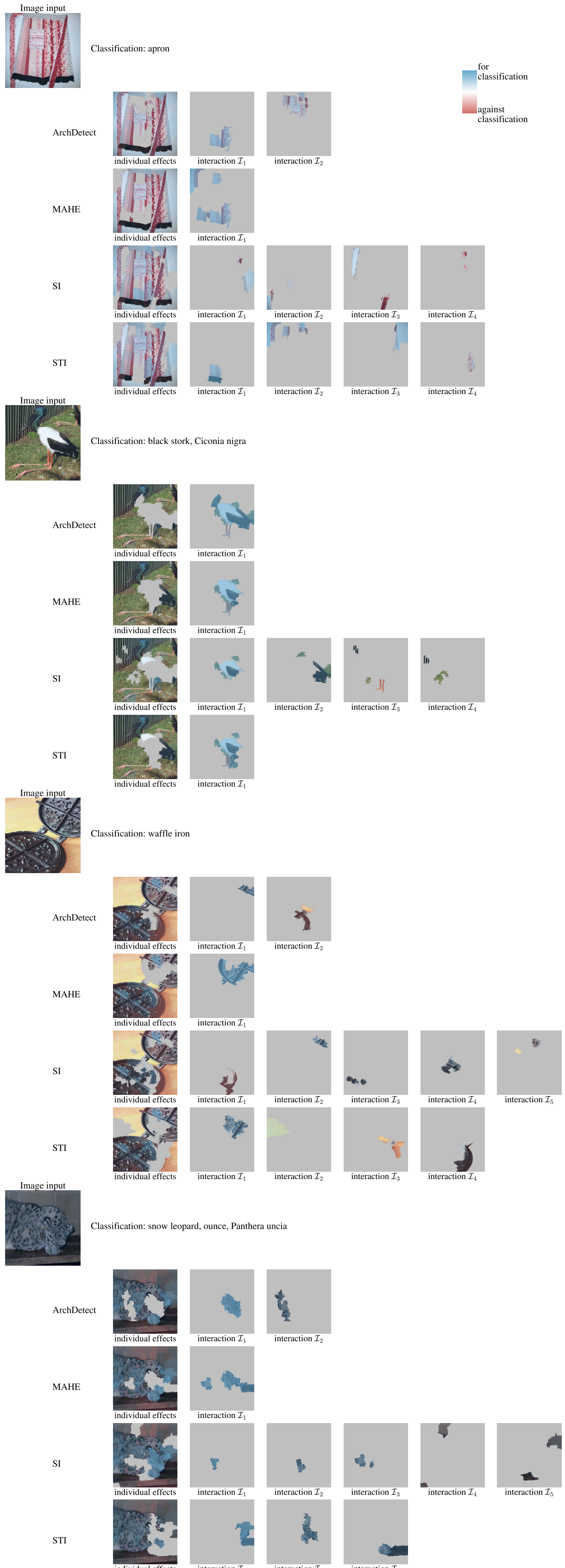


Figure 28: Image Viz. with `ArchAttribute` + Different Interaction Detectors B.

Figure 29: Image Viz. with `ArchAttribute` + Different Interaction Detectors C.