MCCE: MISSINGNESS-AWARE CAUSAL CONCEPT EX-PLAINER

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ABSTRACT

Causal concept effect estimation is gaining increasing interest in the field of interpretable machine learning. This general approach explains the behaviors of machine learning models by estimating the causal effect of human-understandable concepts, which represent high-level knowledge more comprehensibly than raw inputs like tokens. However, existing causal concept effect explanation methods assume complete observation of all concepts involved within the dataset, which can fail in practice due to incomplete annotations or missing concept data. We theoretically demonstrate that unobserved concepts can bias the estimation of the causal effects of observed concepts. To address this limitation, we introduce the Missingness-aware Causal Concept Explainer (MCCE), a novel framework specifically designed to estimate causal concept effects when not all concepts are observable. Our framework learns to account for residual bias resulting from missing concepts and utilizes a linear predictor to model the relationships between these concepts and the outputs of black-box machine learning models. It can offer explanations on both local and global levels. We conduct validations using a real-world dataset, demonstrating that MCCE achieves promising performance compared to state-of-the-art explanation methods in causal concept effect estimation.

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1 INTRODUCTION

Machine learning models explained through concept-based methods are often more intuitive than those based solely on raw inputs like tokens or pixels (Poeta et al., 2023). Unlike traditional approaches that attribute model decisions to low-level features, such as individual pixels in an image or tokens in text, concept-based methods leverage high-level semantic knowledge derived from these inputs. These methods facilitate a deeper understanding of how models make decisions by aligning their internal representations with concepts that are comprehensible to humans. By focusing on high-level concepts, stakeholders can better assess the model's reasoning process. This is especially significant in areas like healthcare (Cutillo et al., 2020; Rasheed et al., 2022) and finance (Giudici & Raffinetti, 2023; Zhou et al., 2022), where trust and transparency are critical.

040 The gold standard for assessing a concept-based explanation is comparing its output to the causal 041 effect of concepts (Wu et al., 2023). Causal effect estimation measures the direct impact of changing 042 a specific concept on the outcome, while holding all other concepts constant. This approach goes 043 beyond simple associations, which are prone to confounding effects, by identifying how altering 044 a specific concept causally influences the model's predictions (Moraffah et al., 2020). However, current concept-based causal explanation methods usually assume that the entire set of involved concepts is completely observed in the dataset. In reality, the identification of concepts from data 046 can vary between experts or automated systems, and one or many concepts may not be annotated 047 in the entire dataset (Ghorbani et al., 2019). As a result, complete observation and annotation of all 048 relevant concepts are not guaranteed in real-world applications, highlighting the need for methods that can handle incomplete or missing concept data. 050

In this paper, we conduct a mathematical analysis showing that the presence of unobserved concepts hinders the unbiased estimation of concepts' causal effects. To address this challenge, we propose a framework called Missingness-aware Causal Concept Explainer (MCCE). MCCE captures the impact of unobserved concepts by constructing pseudo-concepts that are orthogonal to observed

concepts. By modeling the relationship between concepts and a black-box model's output with a linear function, MCCE can not only estimate causal concept effects for individual samples (local explanation) and but also elucidate general rules used by a model to make decisions (global explanations). MCCE can also function as an interpretable prediction model if trained with groundtruth labels. The architecture of MCCE is depicted in Figure 1.



Figure 1: The architecture of MCCE. Given an input sample, a vector representation is extracted.
Pseudo-concepts are constructed under the constraint that they are orthogonal to the observed concepts, ensuring that the pseudo-concepts offers information to compensate for any lost information
from unobserved concepts. Then a linear predictor is trained on the concatenation of observed
concepts and the pseudo-concepts to approximate the behaviors of a black-box model. The entire
pipeline can be trained end-to-end.

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We summarize our main contributions as follows:

- We demonstrate that violating the assumption of complete observation of concepts, which is commonly imposed in existing research, can lead to biased estimation of causal concept effects.
- We propose the Missingness-aware Causal Concept Explainer (MCCE), to our best knowledge, the first concept-based causal effect estimation framework that takes the existence of unobserved concepts into consideration.
- Empirical results show that our proposed MCCE achieves promising performance in estimating the Individual Concept Causal Effect Errors (ICaCE-Error) on a real-world dataset. Meanwhile, it can provide global interpretations of a model and can act as an interpretable white-box prediction model.

2 RELATED WORK

Explaining the behaviors of black-box machine learning models has been drawing interest from 098 researchers in the past decade. Various methods have been proposed to estimate the contribution of input to models' output. Learned weights can be used to denote the importance of features (Olden & Jackson, 2002; Zhou et al., 2016; Molnar, 2020). Permutation-based methods evaluate 100 feature importance by measuring how the model's prediction performance changes when the values 101 of a single feature are randomly shuffled (Altmann et al., 2010; Lundberg, 2017; Smith et al., 2020). 102 Gradient-based methods interpret machine learning models by analyzing the gradients of the model's 103 output with respect to its input (Sundararajan et al., 2017; Kim et al., 2018; Srinivas & Fleuret, 2020). 104 However, these approaches focus on individual input features instead of summerizing the effect of 105 high-level semantic concepts. 106

107 The concept-based explanation uses high-level semantic concepts to interpret a black-box machine learning model's behaviors. Koh et al. (2020) introduced the Concept Bottleneck Model, which

108 predicts human-interpretable concepts as intermediate variables first and then uses these predicted 109 concepts to make final predictions with an interpretable model such as a linear regression. Since 110 then, variants of approaches have been developed to build concept-based interpretation frameworks, 111 such as Concept Transformer (Rigotti et al., 2021), Post-hoc Concept Bottleneck Models (Yuksek-112 gonul et al., 2022), Concept Embedding Models (Zarlenga et al., 2022), Logic Explained Networks (Ciravegna et al., 2023), Probabilistic Concept Bottleneck Models (Kim et al., 2023), Enerby-based 113 Concept Bottleneck Models (Xu et al., 2024), among others. 114

115 Recent years have witnessed the rising interests in causal concepts effect estimation. Feder et al. 116 (2021) proposed CausalLM to estimate concept-based causal effects by learning counterfactual rep-117 resentations via adversarial tasks. Ravfogel et al. (2020) introduced Iterative Nullspace Projection 118 to learn the causal effect of a concept, which removes a concept from a representation vector by iteratively training linear classifiers to predict the attribute and projecting it onto the null space. 119 Abraham et al. (2022) not only built a human-validated concept-based dataset with counterfactuals 120 called Causal Estimation-Based Benchmark (CEBaB) but also found that many popular explanation 121 methods, including those described above, can fail to accurately estimate the causal effects of models 122 on their developed dataset. Wu et al. (2023) developed the Causal Proxy Model (CPM) which mim-123 ics the counterfactual behaviors of a model by creating representations that allow for intervention, 124 achieving state-of-the-art performance on the CEBaB dataset. However, their approach assumes all 125 the involved concepts are observed during the development process. Our work provides a theoretical 126 analysis of the impact of unobserved concepts and, motivated by this analysis, proposes a solution 127 to reduce the resulting bias. We also compare the accuracy of causal effect estimation using our 128 proposed method against existing approaches on the CEBaB dataset.

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3 MISSINGNESS-AWARE CONCEPT-BASED CAUSAL EXPLAINER

132 In this section, we introduce the problem settings, analyze the impact of unobserved concepts on the concepts' causal effect estimation, and provide detailed descriptions of the proposed MCCE.

Causal structure Let U be the exogenous variable, C_{ob} be the observed concepts, C_{un} be the 135 unobserved concepts, X be the input data fed to a black-box model \mathcal{N} , and $\mathcal{N}(X)$ be the output of 136 the model. The exogenous variable U represents the complete state of the world. The input data X137 is generated from U and mediated by concepts C_{ob} and C_{un} . A black-box machine learning model 138 $\mathcal N$ takes the input X and makes output for a specific prediction task. Figure 2 shows the causal 139 structure in a graph as an illustration. 140



153 Figure 2: Causal structure graph. The impact of U on X is not only mediated by the observed 154 concepts $C_{ob_1}, ..., C_{ob_k}$ but also by the unobserved concepts $C_{un_1}, ..., C_{un_j}$. In this work, we aim to 155 account for the impact of unobserved concepts when estimating the causal effect of observed concepts, which has not been addressed in existing research. A backdoor path may exist from C_{ob_1} 156 to $\mathcal{N}(X)$, even though there is no direct path from C_{ob_1} to $\mathcal{N}(X)$ and all other C_{ob} are condi-157 tioned/blocked – this occurs through U and one of C_{un} (Pearl, 2009). 158

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Empirical Individual Concept Causal Effect (ICaCE) Let x^c denote an input sample with a 160 concept value equal to c. For a black-box model \mathcal{N} , the empirical individual causal concept effect 161 (Abraham et al., 2022) of changing the value of concept C from c to c' on input x is denied as

$$\widehat{\text{ICaCE}}_{\mathcal{N}}(x^{c \to c'}) = \mathcal{N}(x^{c \to c'}) - \mathcal{N}(x^c)$$
(1)

ICaCE measures how perturbing a specific concept in a black-box model impacts the prediction of
 a specific input sample.

ICaCE-Error For a black-box model \mathcal{N} , a dataset D, and a distance metric Dist, the ICaCE-Error (Abraham et al., 2022) of an explanation method \mathcal{E} for swapping the value of concept C from c to c' is

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173 174 $ICaCE-Error_{\mathcal{N}}(\mathcal{E}) = \frac{1}{|D|} \sum_{x^c \in D} \text{Dist}\left(\widehat{ICaCE}_{\mathcal{N}}(x^c, x^{c \to c'}), \mathcal{E}(c, c'|x)\right)$ (2)

175 ICaCE-Error measures the average distance between the ICaCE and the estimation returned by ex-176 plainer \mathcal{E} across samples with concept value c. It is used as the quantitative evaluation metric for 177 causal concept effect explanations (Abraham et al., 2022; Wu et al., 2023).

Explaining causal concept effect with a linear model We assume that there exists a linear explainer \mathcal{E}^* for the **complete** concept set $C_{complete}$ that can perfectly explain the logit output of the $\mathcal{N}(X)$ with coefficients β^* :

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$$\mathcal{E}^* = C_{complete}^T \beta^* = \mathcal{N}(X) \tag{3}$$

This linear assumption has been imposed by existing concept-based model explanation frameworks.
 Empirically, it can often hold approximately within concept-based explanation, as concepts tend to have proportional influences on the outcome across different scenarios. (Kim et al., 2018; Yuksek-gonul et al., 2022; Tan et al., 2024).

Suppose we have an input sample x with its tth concepts swapping from value c to value c'. β_t^* is the corresponding coefficient for the tth concept in Equation 3. Because all the remaining concepts are not changed, the ICaCE can be rewritten as

 $\widehat{\text{ICaCE}}_{\mathcal{N}}(x^{c \to c'}) = \mathcal{N}(x^{c \to c'}) - \mathcal{N}(x^{c})$ $= (c' - c)\beta_{t}^{*}$ (4)

For a linear explanation \mathcal{E} with coefficients $\hat{\beta}$, the ICaCE-Error can be written as

$$\begin{aligned} \text{ICaCE-Error}_{N}(\mathcal{E}) &= \frac{1}{|D|} \sum_{x^{c} \in D} \text{Dist}\left(\widehat{\text{ICaCE}}_{\mathcal{N}}(x^{c}, x^{c \to c'}), \mathcal{E}(c, c'|x)\right) \\ &= \frac{1}{|D|} \sum_{x^{c} \in D} \text{Dist}\left(\beta_{t}^{*}(c'-c), \hat{\beta}_{t}(c'-c)\right) \\ &\propto \sum_{x^{c} \in D} \text{Dist}\left(\beta_{t}^{*}, \hat{\beta}_{t}\right) \end{aligned}$$
(5)

That being said, to minimize the ICaCE-Error, one needs to find unbiased estimators for the linear coefficients β^* . This is feasible with regular estimators such as an mean squared error (MSE) when all the involved concepts $C_{complete}$ are observed.

Residual bias resulted from unobserved concepts Complete observation is rarely available in real life. We write $C_{complete} = [C_{ob}, C_{un}]$ as the concatenation of observed concepts C_{ob} and unobserved concepts C_{un} . We want to find $\hat{\beta}_{ob}$ for

$$\mathcal{N}(X) = C_{ob}^T \hat{\beta}_{ob} + C_{un}^T \hat{\beta}_{un} \tag{6}$$

where $\mathcal{N}(X) = C_{ob}^T \beta_{ob}^* + C_{un}^T \beta_{un}^*$.

The existence of residue $C_{un}^T \beta_{un}^* - C_{un}^T \hat{\beta}_{un}$ hinders the unbiased estimation of β_{ob}^*

218 Missingness-aware Concept-based Causal Explainer (MCCE)

The core idea behind MCCE is to compensate for information missed in observed concepts C_{ob} by harnessing the raw input data. We create vectors, termed pseudo-concepts (denoted as C_{pseud}), that are orthogonal to the observed concept vectors using linear transformations from encoded input data. These pseudo-concepts are then combined with the observed concepts to train a linear model that approximates the output of a black-box model. The orthogonality of the pseudo-concepts to the observed concepts prevents collinearity, ensuring that these pseudo-concepts contribute information absent in the observed data.

Suppose C_{ob} is a $n \times k$ vector and C_{pseud} is a $n \times j$ vector, where n is the sample size, k is the number of observed concepts, and j is a hyperparameter to denote the presumed number of pseudo-concepts. An extractor $\mathcal{M}(X)$ takes input X and outputs a $n \times j$ dimensional vector H. We hypothesize that H contains all necessary information about all concepts, including unobserved ones. To capture information from H that is orthogonal to C_{ob} , we rewrite C_{pseud} as below, inspired by recent work in factor analysis (Fan et al., 2024)

$$C_{pseud} = (I - P)H \tag{7}$$

where I is the identification matrix and $P = C_{ob}(C_{ob}^T C_{ob})^{-1}C_{ob}^T$ is the orthogonal projection matrix onto the column space of C_{ob} . (I-P)H denotes the residuals of H after projecting onto the column space of C_{ob} . We have $C_{ob}^T C_{pseud} = 0$ because

$$C_{ob}^{T}C_{pseud} = C_{ob}^{T}(I - P)H$$

$$= (C_{ob}^{T} - C_{ob}^{T}P)H$$

$$= (C_{ob}^{T} - C_{ob}^{T})H \quad \text{since } C_{ob}^{T}P = C_{ob}^{T} \text{ by defination}$$

$$= 0$$
(8)

With C_{ob} and C_{pseud} , we construct a linear predictor $\mathcal{N}(X)$:

$$\mathcal{N}(X) = C_{ob}^T \hat{\beta}_{ob} + C_{pseud}^T \hat{\beta}_{pseud} \tag{9}$$

We plug in Equation 7 to an MSE estimator to find $\hat{\beta_{ob}}$ such that

$$(\hat{\beta}_{ob}, \hat{\beta}_{pseud}) = \underset{\beta_{ob}, \beta_{pseud}}{\arg\max} \left(\frac{1}{2n} ||\mathcal{N}(X) - C_{ob}^T \beta_{ob} - (I - P)H \beta_{pseud}||_2^2 \right)$$
(10)

As a summary, our proposed MCCE converts input to a numerical vector and transforms this vector into pseudo-concepts that are orthogonal to the observed concepts. Then a linear predictor is used to approximate a black-box model's output using the observed concepts and the pseudo-concepts. Let $C_{x,ob}$ denote the observed concept vector of input x, the linear predictor \mathcal{G} can be written as:

$$\mathcal{G}(C_{x,ob}, x, \mathcal{M}) = C_{x,ob}^T \hat{\beta}_{ob} + \left[\left(I - C_{x,ob} (C_{x,ob}^T C_{x,ob})^{-1} C_{x,ob}^T \right) \mathcal{M}(x) \right]^T \hat{\beta}_{pseud}$$
(11)

To estimate the causal effect of a concept swapping from c to c' in the inference stage, we intervene the corresponding values in C_{ob} , with x remaining unchanged. With $C_{x,ob}^{c \to c'}$ denoting swapping one of input x's concepts from c to c', the MCCE explainer \mathcal{E}_{MCCE} can be written as:

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$$\mathcal{E}_{MCCE}(c,c'|x) = \mathcal{G}_{\mathcal{M}}(C^{c,\to c'}_{x,ob}, x) - \mathcal{N}(x)$$
(12)

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270 4 EXPERIMENTS

272 4.1 DATASET 273

We use the CEBaB dataset Abraham et al. (2022) to validate our proposed MCCE. CEBaB contains 274 restaurant reviews from OpenTable for sentiment analysis. Each text in CEBaB received a 5-star sen-275 timent score from crowd workers and was annotated on four concept levels-ambiance, food, noise, 276 and service, with the labels negative, unknown, and positive. It started with 2,299 original reviews and was expanded to 15,089 texts through modifications by human annotators. These annotators 278 edited the reviews to reflect specific interventions such as changing food evaluations from positive 279 to negative. As far as we know, it is the only dataset with human-verified approximate counterfac-280 tual text. The resulting dataset is divided into training, development, and testing partitions. The 281 development and test sets serve to evaluate explanation methods. The ICaCE-Error of MCCE and 282 the baselines are validated using the test set. 283

4.2 MCCE CONSTRUCTION

We finetune three different types of publicly available models for the multiclass semantic classifica-286 tion tasks of the CEBaB dataset: the base BERT (Devlin, 2018), the base RoBERTa (Liu, 2019), and 287 Llama-3 (Dubey et al., 2024). These three models are different generations of transformer-based 288 language models designed to capture contextual relationships within text and have been widely used 289 in a wide range of NLP tasks. We use the last hidden states of the *cls* token for BERT and RoBERTa 290 as the H vector in Equation 7, and for Llama-3, we use the last hidden states of the last token. To 291 explore how unobserved concepts influence the ICaCE-Error across different explainers, we omit 292 each of the four attributes individually during the construction of MCCE and the baseline models. 293 Additionally, we exclude every possible pair of concepts from these four attributes.

4.3 BASELINES

Let x^c denote an input sample with a concept value c. We implement below methods as baselines to estimate the ICaCE-Error of swapping a concept value from c to c' for a black-box model \mathcal{N} .

Approximate Counterfactuals As a baseline, we sample a factual input with the same concept labels as the $x_{sampled}^{c'}$ and use it as an approximate counterfactual. This approximate counterfactuals explainer can be formally written as

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 $\mathcal{E}_{approx}(c,c'|x) = \mathcal{N}(x_{sampled}^{c'}) - \mathcal{N}(x^c)$ (13)

S-Learner The S-Learner, originally proposed for Conditional Average Treatment Effect (CATE) estimation (Künzel et al., 2019), is one of the top performers in the original CEBaB paper. It uses all the observed concepts to fit a logistic regression model \mathcal{R} to predict the output of \mathcal{N} . At the inference stage, it compute the difference between the counterfactual concept vector $C_{x,ob}^{c \to c'}$ and the factual concept vector $C_{x,ob}^{c}$

$$\mathcal{E}_{S-Learner}(c,c'|x) = \mathcal{R}(C_{x,ob}^{c \to c'}) - \mathcal{N}(x^c)$$
(14)

Input-based Causal Proxy Model The input-based Causal Proxy Model (CPM) (Wu et al., 2023) outperforms existing approaches on the CEBaB dataset. Given a counterfactual pair $(x^{c \to c'}, x^c)$, where $x^{c \to c'}$ is the human-created counterfactual sample, CPM concatenates a learnable token $tk_{c \to c'}$ to the end of the original text x^c and train a language model \mathcal{P} , which shares the same architecture as the black-box model \mathcal{N} , to approximate the output of \mathcal{N} with the counterfactual input by minimizing the smoothed cross-entropy (Hinton, 2015) as:

$$\mathcal{L}_{CPM} = CE\left(\mathcal{N}(x^{c \to c'}), \mathcal{P}(x^{c}, tk_{c \to c'})\right)$$
(15)

During the inference stage, the CPM measures the causal concept effect of swapping c to c' as the difference between $\mathcal{P}(x^c, tk_{c \to c'})$ and the black-box model's factual output $\mathcal{N}(x^c)$. The CPM explainer \mathcal{E}_{CPM} can be written as
$$\mathcal{E}_{CPM}(c,c'|x) = \mathcal{P}(x^c, tk_{c \to c'}) - \mathcal{N}(x^c)$$
(16)

RESULTS

We conduct validation of MCCE alongside baseline methods using the CEBaB dataset. Table 1 reports the means and standard deviations of the ICaCE-Error when two concepts or one concept are unobserved. For a specific number of unobserved concepts, the means and standard deviations of ICaCE-Error are displayed for all possible combinations of unobserved concepts. To assess the ICaCE-Error, we employ L2, Cosine, and Norm distance metrics. MCCE outperforms S-Learner over all the metrics with either one or two concepts being unobserved. As S-Learner only trains a learner predictor with observed concepts, it can be recognized as a special case of MCCE that removed the components of the pseudo-concepts. The contrast between MCCE and S-Learner demonstrates that the capture of pseudo-concepts effectively mitigates the residue bias caused by the unobserved concepts. MCCE consistently achieves performance on par with or superior to the CPM across all considered distance metrics. When two out of the four concepts are unobserved, MCCE demonstrates a distinct advantage over the baselines in terms of Cosine distance, which pri-oritizes the directional alignment between vector pairs rather than merely their magnitude. While CPM accurately estimates causal concept effects by learning the impact of altering a concept value while keeping other elements constant, its performance declines with two concepts are unobserved compared to only one, particularly measured using Cosine distance. On the other hand, MCCE demonstrates robust performance especially when evaluated using Cosine distance, underscoring its effectiveness in mitigating residual bias to estimate the direction of causal concept effect through the construction of pseudo-concepts that are orthogonal to observed concepts.

Table 1: Means and standard deviations of ICaCE-Error (the lower, the better) of MCCE and base-lines with three different types of models when two or one concepts are unobserved in the CEBaB dataset. Best results are bolded. For each number of unobserved concepts, means and standard de-viations for all possible combinations of unobserved concepts are displayed.

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353			Two a	concepts a	re unobse	erved	One o	concepts a	re unobse	erved
354 355	Model	Metric	Approx	S-Learner	CPM	MCCE (ours)	Approx	S-Learner	СРМ	MCCE (ours)
356	BERT	L2	1.52	1.29	1.01	1.02	1.52	1.10	0.98	0.99
357			(0.06)	(0.05)	(0.05)	(0.05)	(0.05)	(0.02)	(0.04)	(0.03)
358		Cosine	0.75	0.64	0.60	0.56	0.75	0.60	0.56	0.57
359			(0.03)	(0.03)	(0.03)	(0.02)	(0.03)	(0.03)	(0.02)	(0.03)
360		Norm	0.88	0.78	0.65	0.66	0.88	0.72	0.64	0.68
361			(0.06)	(0.05)	(0.04)	(0.04)	(0.06)	(0.05)	(0.05)	(0.04)
362	RoBERTa	L2	1.48	1.30	0.99	0.98	1.48	1.15	0.99	0.95
363			(0.06)	(0.04)	(0.05)	(0.04)	(0.06)	(0.03)	(0.04)	(0.04)
364		Cosine	0.72	0.65	0.61	0.57	0.72	0.60	0.57	0.57
365			(0.04)	(0.04)	(0.03)	(0.03)	(0.04)	(0.04)	(0.03)	(0.02)
366		Norm	0.91	0.81	0.64	0.65	0.91	0.73	0.63	0.66
367			(0.05)	(0.05)	(0.04)	(0.05)	(0.05)	(0.05)	(0.05)	(0.04)
368	Llama 3	L2	1.32	0.95	0.81	0.82	1.32	0.90	0.81	0.78
369			(0.05)	(0.03)	(0.03)	(0.04)	(0.05)	(0.03)	(0.04)	(0.04)
370		Cosine	0.64	0.55	0.55	0.50	0.72	0.60	0.57	0.51
371			(0.03)	(0.03)	(0.02)	(0.03)	(0.04)	(0.04)	(0.03)	(0.02)
372		Norm	0.85	0.76	0.58	0.52	0.85	0.70	0.55	0.52
373			(0.03)	(0.05)	(0.02)	(0.05)	(0.03)	(0.03)	(0.05)	(0.02)
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MCCE can offer a global interpretation of the impact each observed concept has on the output of a black-box model. This is demonstrated in Figure 3, which shows the coefficients for the attributes "Ambiance," "Service," and "Noise" in a five-class sentiment classification task. To adhere to the identification constraints required for multiclass classification, we designate the coefficients of the

1-star category as the baseline for comparison. For "Noise" and "Service" with positive attitudes, the coefficient shows increasing positive influence as the ratings increase, becoming most prominent at a 4-star rating. A positive "Ambiance" has a peaking impact at the 5-star rating instead of the 5-star rating. The negative attitudes toward the three attributes result in heavier negative influences on higher ratings. The "*unknown*" category has moderate impacts with smaller magnitudes of coefficients and tends to slightly lean towards mid-class like 3-star ratings. This figure demonstrates MCCE's ability to depict how each attribute's impact varies across different ratings for a given model, which is lacking in the CPM model.

MCCE not only provides causal explanations but also can function as an interpretable predictor. Table 2 displays MCCE's performance, measured by macro-F1 score, when it is used to directly learn sentimental outcomes instead of interpreting a black-box model's output. MCCE predictor achieves comparable performance when leveraging BERT and RoBERTa's hidden states compared to their black-box model counterpart. When leveraging an LLM as the extractor, MCEE only slightly underperforms compared to the Llama-3 black-box model. Notably, the performance of MCCE remains robust, showing only a marginal decrease, when two concepts are unobserved compared to just one. This again demonstrates that the pseudo-concepts can capture critical information that is missed from observed concepts.

		*	**	★★★ Stars	****	****		1.5
	Ambiance_positive -	0	0.0427	0.1131	0.8837	1.0587		1 5
,	Ambiance_unknown -	0	0.1441	0.1494	0.1191	-0.1084		1.0
Ambiance_negative -		0	0.1986	-0.3583	-0.7991	-1.2521		0.:
Attribute	Service_positive -	0	-0.2003	0.4937	1.1973	0.9905		0.5
	Service_unknown -	0	0.07	0.0762	-0.2089	-0.293		- 0.0
	Service_negative -	0	0.2306	-0.432	-1.3393	-1.6044		- 0.5
	Noise_positive -	0	0.0049	0.8846	1.2836	0.9284		0.5
	Noise_unknown -	0	-0.2767	0.038	-0.1973	-0.2656		- 1.0
	Noise_negative -	0	-0.2751	-0.2073	-0.3031	-0.8496		- 1.5
		Coefficients when setting the 1-star as baseline					1 5	

Figure 3: An illustration of the MCCE's global interpretation on a BERT model when the concepts of "Ambiance", "Service", and "Noise" are observed.

Table 2: Macro-F1 (the larger, the better) performance of MCCE on directly predicting the CEBaB outcomes. "1 unobserved" and "2 unobserved" indicate one and two concepts are unobserved. Means and standard deviations for all possible combinations of unobserved concepts are displayed.

Model	Blackbox	MCCE (1 unobserved)	MCCE (2 unobserved)
BERT	0.72 (0.02)	0.72 (0.02)	0.71 (0.02)
RoBER	Ta 0.71 (0.02)	0.72 (0.02)	0.70 (0.03)
Llama-3	0.78 (0.01)	0.75 (0.02)	0.74 (0.02)

432 6 DISCUSSION

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434 In this work, we address a critical but previously unexplored question: How can we effectively mea-435 sure the causal effect of concepts when some are unobserved? We introduce the Missingness-aware 436 Concept-based Causal Explainer (MCCE), the first framework specifically designed to estimate the 437 causal effects of concepts while accounting for the impact of those that are unobserved. MCCE innovatively constructs pseudo-concepts that are column-wise orthogonal to the observed concepts, 438 enriching the model with complementary information that captures the influence of the missing 439 concepts. Our experimental results on the CEBaB dataset demonstrate that MCCE achieves supe-440 rior or, at the very least, comparable performance to existing baseline methods in scenarios where 441 unobserved concepts are present. 442

- Among the baseline methods, the CPM approach is the only one that matches MCCE's performance on some of the metrics. However, CPM methods depend on labeled counterfactual data for training, which may limit their practical applicability. In contrast, MCCE effectively utilizes only factual training data and does not require counterfactual data. Additionally, the coefficients derived from MCCE's linear predictor offer a direct, global interpretation of black-box models, a character absent in CPM.
- The number of pseudo-concepts in MCCE is a hyperparameter that needs to be pre-selected. Empirically, we observe that a number of pseudo-concepts comparable to or slightly greater than the number of observed concepts tends to yield the best results. For example, in a scenario where one of four attributes in CEBaB is unobserved, with the remaining three attributes encoded into nine concepts (*"negative"*, *"unknown"*, *"positive"* for each attribute). MCCE shows optimal performance with nine or twelve pseudo-concepts. The theoretical rationale for the choice of the number of pseudo-concepts remains a subject for further investigation.
- One limitation of our work is that MCCE is validated on one dataset. The CEBaB dataset, which, 456 while comprehensive, contains only a limited number of labeled concepts. Though the construc-457 tion of the orthogonal pseudo-concepts and the linear predictor allows MCCE to cope with a large 458 number of concepts through straightforward modifications according to Fan et al. (2024), further 459 empirical validation is necessary to fully establish its effectiveness across varied datasets. In ad-460 dition, MCCE is designed to be modal-agnostic but needs further validation on modalities beyond 461 text. Unfortunately, to our knowledge, CEBaB is the sole publicly available dataset that includes the 462 labeled counterfactual data necessary for assessing causal concept effects. Further validation will be 463 available only when more benchmark datasets for causal concept effect estimation are available. 464

References

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- Eldar D Abraham, Karel D'Oosterlinck, Amir Feder, Yair Gat, Atticus Geiger, Christopher Potts,
 Roi Reichart, and Zhengxuan Wu. Cebab: Estimating the causal effects of real-world concepts
 on nlp model behavior. *Advances in Neural Information Processing Systems*, 35:17582–17596,
 2022.
- André Altmann, Laura Toloşi, Oliver Sander, and Thomas Lengauer. Permutation importance: a corrected feature importance measure. *Bioinformatics*, 26(10):1340–1347, 2010.
- Gabriele Ciravegna, Pietro Barbiero, Francesco Giannini, Marco Gori, Pietro Lió, Marco Maggini, and Stefano Melacci. Logic explained networks. *Artificial Intelligence*, 314:103822, 2023.
- Christine M Cutillo, Karlie R Sharma, Luca Foschini, Shinjini Kundu, Maxine Mackintosh, Kenneth D Mandl, and MI in Healthcare Workshop Working Group Beck Tyler 1 Collier Elaine 1
 Colvis Christine 1 Gersing Kenneth 1 Gordon Valery 1 Jensen Roxanne 8 Shabestari Behrouz 9
 Southall Noel 1. Machine intelligence in healthcare—perspectives on trustworthiness, explainability, usability, and transparency. *NPJ digital medicine*, 3(1):47, 2020.
- Jacob Devlin. Bert: Pre-training of deep bidirectional transformers for language understanding. *arXiv preprint arXiv:1810.04805*, 2018.
- Abhimanyu Dubey, Abhinav Jauhri, Abhinav Pandey, Abhishek Kadian, Ahmad Al-Dahle, Aiesha
 Letman, Akhil Mathur, Alan Schelten, Amy Yang, Angela Fan, et al. The llama 3 herd of models. arXiv preprint arXiv:2407.21783, 2024.

486 487 488	Jianqing Fan, Zhipeng Lou, and Mengxin Yu. Are latent factor regression and sparse regression adequate? <i>Journal of the American Statistical Association</i> , 119(546):1076–1088, 2024.
489 490	Amir Feder, Nadav Oved, Uri Shalit, and Roi Reichart. Causalm: Causal model explanation through counterfactual language models. <i>Computational Linguistics</i> , 47(2):333–386, 2021.
491 492	Amirata Ghorbani, James Wexler, James Y Zou, and Been Kim. Towards automatic concept-based explanations. <i>Advances in neural information processing systems</i> , 32, 2019.
493 494 495	Paolo Giudici and Emanuela Raffinetti. Safe artificial intelligence in finance. <i>Finance Research Letters</i> , 56:104088, 2023.
496 497 498	Geoffrey Hinton. Distilling the knowledge in a neural network. <i>arXiv preprint arXiv:1503.02531</i> , 2015.
499 500 501	Been Kim, Martin Wattenberg, Justin Gilmer, Carrie Cai, James Wexler, Fernanda Viegas, et al. Interpretability beyond feature attribution: Quantitative testing with concept activation vectors (tcav). In <i>International conference on machine learning</i> , pp. 2668–2677. PMLR, 2018.
502 503	Eunji Kim, Dahuin Jung, Sangha Park, Siwon Kim, and Sungroh Yoon. Probabilistic concept bot- tleneck models. <i>arXiv preprint arXiv:2306.01574</i> , 2023.
505 506 507	Pang Wei Koh, Thao Nguyen, Yew Siang Tang, Stephen Mussmann, Emma Pierson, Been Kim, and Percy Liang. Concept bottleneck models. In <i>International conference on machine learning</i> , pp. 5338–5348. PMLR, 2020.
508 509 510	Sören R Künzel, Jasjeet S Sekhon, Peter J Bickel, and Bin Yu. Metalearners for estimating heteroge- neous treatment effects using machine learning. <i>Proceedings of the national academy of sciences</i> , 116(10):4156–4165, 2019.
512 513	Yinhan Liu. Roberta: A robustly optimized bert pretraining approach. <i>arXiv preprint arXiv:1907.11692</i> , 2019.
514 515 516	Scott Lundberg. A unified approach to interpreting model predictions. <i>arXiv preprint arXiv:1705.07874</i> , 2017.
517	Christoph Molnar. Interpretable machine learning. Lulu. com, 2020.
518 519 520	Raha Moraffah, Mansooreh Karami, Ruocheng Guo, Adrienne Raglin, and Huan Liu. Causal inter- pretability for machine learning-problems, methods and evaluation. <i>ACM SIGKDD Explorations</i> <i>Newsletter</i> , 22(1):18–33, 2020.
522 523 524	Julian D Olden and Donald A Jackson. Illuminating the "black box": a randomization approach for understanding variable contributions in artificial neural networks. <i>Ecological modelling</i> , 154 (1-2):135–150, 2002.
525	J Pearl. Causality. Cambridge university press, 2009.
520 527 528	Eleonora Poeta, Gabriele Ciravegna, Eliana Pastor, Tania Cerquitelli, and Elena Baralis. Concept- based explainable artificial intelligence: A survey. <i>arXiv preprint arXiv:2312.12936</i> , 2023.
529 530 531 532	Khansa Rasheed, Adnan Qayyum, Mohammed Ghaly, Ala Al-Fuqaha, Adeel Razi, and Junaid Qadir. Explainable, trustworthy, and ethical machine learning for healthcare: A survey. <i>Computers in Biology and Medicine</i> , 149:106043, 2022.
533 534	Shauli Ravfogel, Yanai Elazar, Hila Gonen, Michael Twiton, and Yoav Goldberg. Null it out: Guard- ing protected attributes by iterative nullspace projection. <i>arXiv preprint arXiv:2004.07667</i> , 2020.
535 536 537 538	Mattia Rigotti, Christoph Miksovic, Ioana Giurgiu, Thomas Gschwind, and Paolo Scotton. Attention-based interpretability with concept transformers. In <i>International conference on learning representations</i> , 2021.
539	Gavin Smith, Roberto Mansilla, and James Goulding. Model class reliance for random forests. <i>Advances in Neural Information Processing Systems</i> , 33:22305–22315, 2020.

540 541	Suraj Srinivas and François Fleuret. Rethinking the role of gradient-based attribution methods for model interpretability. <i>arXiv preprint arXiv:2006.09128</i> , 2020.
542 543	Mukund Sundararajan, Ankur Taly, and Qiqi Yan. Axiomatic attribution for deep networks. In <i>International conference on machine learning</i> , pp. 3319–3328. PMLR, 2017.
545 546 547	Zhen Tan, Tianlong Chen, Zhenyu Zhang, and Huan Liu. Sparsity-guided holistic explanation for llms with interpretable inference-time intervention. In <i>Proceedings of the AAAI Conference on Artificial Intelligence</i> , volume 38, pp. 21619–21627, 2024.
548 549 550 551	Zhengxuan Wu, Karel D'Oosterlinck, Atticus Geiger, Amir Zur, and Christopher Potts. Causal proxy models for concept-based model explanations. In <i>International conference on machine learning</i> , pp. 37313–37334. PMLR, 2023.
552 553 554	Xinyue Xu, Yi Qin, Lu Mi, Hao Wang, and Xiaomeng Li. Energy-based concept bottleneck models: Unifying prediction, concept intervention, and probabilistic interpretations. In <i>The Twelfth International Conference on Learning Representations</i> , 2024.
555 556 557	Mert Yuksekgonul, Maggie Wang, and James Zou. Post-hoc concept bottleneck models. <i>arXiv</i> preprint arXiv:2205.15480, 2022.
558 559 560 561	Mateo Espinosa Zarlenga, Pietro Barbiero, Gabriele Ciravegna, Giuseppe Marra, Francesco Gian- nini, Michelangelo Diligenti, Zohreh Shams, Frederic Precioso, Stefano Melacci, Adrian Weller, et al. Concept embedding models: Beyond the accuracy-explainability trade-off. <i>arXiv preprint</i> <i>arXiv:2209.09056</i> , 2022.
562 563 564	Bolei Zhou, Aditya Khosla, Agata Lapedriza, Aude Oliva, and Antonio Torralba. Learning deep features for discriminative localization. In <i>Proceedings of the IEEE conference on computer vision and pattern recognition</i> , pp. 2921–2929, 2016.
566 567 568 569	Jun Zhou, Chaochao Chen, Longfei Li, Zhiqiang Zhang, and Xiaolin Zheng. Finbrain 2.0: when finance meets trustworthy ai. <i>Frontiers of Information Technology & Electronic Engineering</i> , 23 (12):1747–1764, 2022.
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