Principles from Clinical Research for NLP Model Generalization

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Abstract

The NLP community typically relies on performance of a model on a held-out test set to assess generalization. Performance drops observed in datasets outside of official test sets are generally attributed to "out-of-distribution" effects. Here, we explore the foundations of generalizability and study the various factors that affect it, articulating generalizability lessons from clinical studies. In clinical research, generalizability depends on (a) *internal validity* of experiments to ensure controlled measurement of cause and effect, and (b) *external validity* or transportability of the results to the wider population. We present the need to ensure internal validity when building machine learning models in natural language processing, especially where results may be impacted by spurious correlations in the data. We demonstrate how spurious factors, such as the distance between entities in relation extraction tasks, can affect model internal validity and in turn adversely impact generalization. We also propose to adapt the idea behind randomized controlled trials to model evaluation in NLP.

1 Introduction

What factors lead to poor generalizability? To understand the causes of non-generalization, the notion of generalizability needs to be first clearly defined. One definition of generalizability, in the context of general machine learning, is the ability of a model to perform well on data *unseen during training*, but *drawn from the same distribution or population* (Google, 2022). Data *unseen during training* clearly refers to data that is not part of training data, and is arguably uncontroversial to support sound evaluation. However, the requirement of data *drawn from the same distribution or population* warrants more scrutiny.

It is important to consider the impact of data distribution on generalization, yet this is very challenging in the context of natural language data. In statistics, the concept of distribution indicates "the pattern of variation in a variable or set of variables in the multivariate case", and thus describes the frequency of values of an observed variable (Wild, 2006). Distribution or frequency of observed variable values can be a challenging notion to meaningfully adapt to high dimensional, multivariate, and high variability inputs such as texts in NLP tasks. Currently, no formal definition of in-distribution or out-of-distribution (OOD) texts, or how to detect them, exists for NLP (Arora et al., 2021). Where distributions are considered, simple surface linguistic characteristics or lexical-level distributions are emphasized (Verspoor et al., 2009).

Despite the lack of a comprehensive formal definition of OOD in existing NLP literature, OOD has become the most commonly cited reason for generalization failure when a model performs poorly outside an official test set. Due to the black-box nature of deep learning models, it is increasingly difficult to demonstrate if a model has established a robust decision-making process that is generalizable to unseen data. As a consequence, generalization failures are typically ascribed to external factors, i.e. those extraneous to model development practices, and primarily to shifts in data distribution, or OOD.

Recent studies have emerged showing that the robustness of a model can also be undermined by inadvertent errors occurring during development of a model. For example, it has been shown that data leakage from training to test splits can lead to inflated results on test sets (Elangovan et al., 2021). Several other works have also pointed out spurious correlations in various benchmark datasets, which can be potentially leveraged by deep learning models to achieve inflated performances on test sets, while having poor generalization capability to real-world datasets (Gururangan et al., 2018; McCoy et al., 2020; Shinoda et al., 2022).

In this paper, we hope to draw attention to the causes of NLP model generalization failures, es-

pecially those internal factors that are part of the model development process (e.g. preparation of training data). We argue that the external validity of a model should only be examined if the internal validity of the model is established. We start with a case study, showing how generalization failures can be caused by internal factors – the model has learned surface patterns in training data. We then propose that a pragmatic notion of model generalizability in the NLP domain can be established through borrowing and adapting practices from a domain seemingly far afield – clinical research.

The contribution of this paper is two-fold. First, we show how OOD may not be the sole cause of generalization failures, via a relation extraction task, highlighting the need for intrinsic investigation of why models fail. Second, we propose to categorize the causes of generalization failures in NLP models, drawing inspiration from clinical studies. Our work provides guidance on how to more systematically analyze generalization failures and adapt the principles behind randomized controlled trials for NLP model evalution.

2 Relation extraction case study

Through a relation extraction case study over two data sets, we demonstrate that poor generalization in real-world application can result from ineffective modelling, *i.e.* learning of superficial surface patterns, rather than data distribution effects.

2.1 Approach

Due to the black-box nature of deep learning models, it is difficult to interpret the underlying basis for model predictions. Inspired by recent works in explainable NLP models, such as LIME (Ribeiro et al., 2016), we employ interpretable surrogate models to examine the behavior of deep learning models. Specifically, we train two surrogate models: a model S_g that is fit on the dataset $\langle x_u, y \rangle$ and another model $S_{\hat{m}}$ that is fit on the dataset $\langle x_u, \hat{y}_m \rangle$, where x_u is a vector of surface patterns used to represent the input sample x, y is the ground truth label, and $\hat{y}_m$ is the prediction of the deep learning model to be examined B_m, e.g. a BERT-based model (Devlin et al., 2019). We hypothesize that if the predictions of the surrogate $S_{\hat{m}}$ has strong correlation with the corresponding main model's prediction, then is likely to be a flag or indicator that the underlying model B_m has relied on the surface patterns in x_u and that the model's predictions may not be reliable. The correlation between the predictions of $S_{\hat{g}}$ and the ground truth labels indicate the extent to which the surface patterns x_u are present in the underlying data, and a strong correlation indicates the weakness in the dataset itself and how these patterns can be exploited to achieve highly accurate predictions without deeper linguistic comprehension. We use Cohen's Kappa κ to measure the correlations and use the stricter limits defined by McHugh (2012) to interpret the correlation as weak, moderate or strongly correlated.

2.2 Datasets

We use two annotated corpora in the experiments:

- **PTM-PPI** is sampled from PubMed abstracts (Elangovan et al., 2022), annotated with 6 types of post-translational modification relationship between two proteins. Out of the 6 positive classes, we only consider the class "phosphorylation" since only this class has a sufficient number (> 100) of training samples. Consequently, the dataset used has 2 classes: "phosphorylation" class and the negative class.
- **ChemProt (CHM-PRT)** is sampled from PubMed abstracts, annotated with 5 types of protein–chemical relationships (Krallinger et al., 2017). The dataset contains 6 classes in total: 5 positive classes and the negative class.

2.2.1 Evaluation data sets

We fine-tune the BioBERT model (Lee et al., 2019) on 2 different relation extraction tasks **(a)** PTM-PPI (Elangovan et al., 2022) and **(b)** ChemProt dataset (Krallinger et al., 2017) using the official training sets. We aim to analyze the trained BioBERT model and validate if it has primarily learned surface patterns, by using surrogate models. In order to understand the generalization behavior of the fine-tuned BioBERT model, we created two additional data sets as described below.

For the first additional dataset, we retain the input samples from the official test set, but replace the original labels with the predictions of the fine-tuned BioBERT model. For the second additional dataset, we select a random subset of PubMed abstracts to create a "generalization" set, and apply the fine-tuned BioBERT model to generate labels. From this generalization set, we randomly sample from the top 25 percentile of the high confidence predictions (set GH) for each class (Elangovan et al.,

Corpus	Dataset (Label)	# Pos / # Neg
PTM-PPI	TR (GT)	139 / 1116
	TS (GT)	44 / 308
	TS (BP)	24 / 328
	GH (BP)	250 / 5000
CHM-PRT	TR (GT)	4172 / 2265
	TS (GT)	3469 / 2275
	TS (BP)	3726 / 2018
	GH (BP)	7500 / 2500

Table 1: Summary of data sets. TR: official training set; GT: ground-truth labels are used; TS: official test set; BP: BioBERT predictions are used as labels; GH: generalization set with high confidence predictions.

2022) and report results across 10 runs. Selecting only the high confidence predictions is inspired by Hendrycks and Gimpel (2017), which demonstrated that the prediction probabilities of OOD samples tend to be lower than those of correct samples. Table 1 summarizes the number of positive and negative samples in all data sets for the two corpora.

2.3 Surrogate models and surface patterns

We employ two explainable surrogate models:

- **Multinomial Naive Bayes (NB)**: The Multinomial Naive Bayes approach represents input samples using simple surface patterns (n-grams, $n = 1$). To avoid over-fitting, we select the top k most commonly n-grams per class. Hence, the maximum number of n-grams that the NB model uses is $k\times$ number of classes. We set k as 100 in the experiment.
- **Naive Bayes + Decision Tree (NB-T)**: Here we use model stacking, where a Decision Tree is stacked on top of a NB model. In NB-T, the prediction of NB is used as one feature input in the subsequent decision tree. Additionally, handcrafted rules, detailed in section 2.3.1, are used as surface pattern features in the decision tree. In order to void over-fitting and to allow the decision process to be explainable, we restrict the tree depth to $<= 4$.

2.3.1 Crafted surface pattern features

In order to study whether the BioBERT-based model has relied on distance-based surface patterns for relation extraction, we manually analyze BioBERT's predictions on the PTM-PPI task and identify 4 surface patterns that potentially explain the model predictions. We then use these handcrafted surface patterns to represent the inputs to a surrogate model and verify how well the predictions of the surrogate model correlates with BioBERT's predictions (which is given the full-text input). The 4 surface patterns are:

- **Percentage count of participating entities (E1C and E2C) :** Given an input sentence s and a relation $\langle E1, Rel, E2\rangle$ in s, this feature captures the percentage of the total tokens in s corresponding to each entity. For instance, for the input *"GENE_A interacts with CHEMICAL_C and binds to CHEMICAL_C and CHEMICAL_D"* and the relation ⟨CHEMICAL_C, Rel, GENE_A⟩, the features E1C and E2C are $\frac{2}{10} * 100 = 20.0$ and $\frac{1}{10} * 100 = 10.0$, respectively (input contains 10 words, E1 occurs twice and E2 once).
- **Length of shortest span containing the participating entities and a given trigger word T (LSS_⟨T⟩):** This feature represents the length of the shortest span containing the two entities and a specified trigger word. For instance, an input *"GENE_A interacts with CHEMICAL_C and binds to CHEMICAL_C and CHEMICAL_D"* and ⟨CHEMICAL_C, Rel, GENE_A⟩ the length of the shortest span containing the trigger word "interacts", LSS_interacts, is 4, whereas LSS_binds is 6.
- **Length of shortest span that contains the entities and any trigger word (LSS):** For instance, given input *"GENE_A interacts with CHEMICAL_C and binds to CHEMICAL_C and CHEMICAL_D"* and relation ⟨CHEMICAL_C, Rel, GENE_A⟩, the shortest span has length 4.
- **Fraction of sentences containing participating entity pair (SPC):** This feature represents the normalized count of sentences containing the entity pair. For instance, if the input text contains s_n sentences and only k sentences contain both entities E1 and E2 in $\langle E1, Rel, E2\rangle$, then this feature would be $\frac{k}{s_n}$.

2.4 Results

Table 2 reports the Kappa correlation between **(a)** the surrogate models and ground truth **(b)** the surrogate models and BioBERT's model prediction for the two corpora. For the PTM corpus, NB-T achieves better correlation with ground-truth, compared to NB, in all settings, demonstrating that the

hand-crafted surface patterns are more likely than just the n-grams to be influencing the model predictions. In addition, when the ground-truth labels are used as targets, i.e. TS (GT) *vs* S_g^{test} predictions and TR (GT) *vs* S_g^{Train} predictions, NB-T correlation κ is 0.55 and 0.54 respectively, indicating that similar surface patterns exist in both the training and test sets of ground-truth labels. This is not surprising given that the test and train sets were obtained using a random split from a single dataset.

To examine if the fine-tuned BioBERT model has relied on those hand-crafted surface patterns, we compare the correlation between NB-T on the test set when fitting to the ground-truth labels, TS (GT), versus the BioBERT predictions, TS (BP). We see that the κ correlation increases drastically from 0.55 – weak correlation, to 0.73 – moderate correlation (based on McHugh (2012) ranges), when the target labels are replaced with BioBERT predictions (cf. trees in Appendix A). This demonstrates that NB-T using handcrafted features is more correlated with BioBERT's predictions compared to ground-truth labels themselves, increasing the evidence that the BioBERT model may rely on these features. This phenomenon is further exacerbated on the GH set, where NB-T achieves κ correlation of 0.85 - strong correlation when fitting to BioBERT's predictions. In fact, Elangovan et al. (2022) report that only 6 out of 30 (20%) of the phosphorylation predictions turned out to be accurate when the high confidence predictions were randomly sampled and verified by experts, compared to test set precision of 62.5%. The drop in precision, compared to test set performance, *may be* explained by the model relying on these surface patterns rather than broadly generalizable features.

In the ChemProt dataset, distance based surface patterns do not seem to be a stronger predictor than n-grams, as shown in Table 2. All the surrogate models have a correlation between 0.4 and 0.5 indicating weak correlation (McHugh, 2012).

OOD is NOT always a sufficient explanation for generalization failures. Given the broad and generic definition of OOD, almost any sample can be categorized as OOD. It is difficult to counter the OOD argument, as there is no comprehensive approach to establishing that a given instance is in-distribution (Arora et al., 2021). While in the case of ChemProt we were unable to detect clear surface

DS (L)	M	PTM κ	CHM κ
TR (GT)	NB	0.33	0.44
	NB-T	0.54	0.43
TS (GT)	NB	0.26	0.42
	NB-T	0.55	0.42
TS (BP)	NB	0.25	0.50
	NB-T	**0.73**	0.50
GH (BP)	NB	0.77 (0.3)	0.44 (0.002)
	NB-T	**0.85** (0.3)	0.44 (0.002)

Table 2: Surrogate model correlations in PTM-PPI (PTM) and ChemProt (CHM) dataset (DS) and the target label (L): The surrogate model (M) NB-T correlates better with BioBERT's prediction than the ground truth labels for the PTM dataset. For GH set, we report standard error for 10 runs ($\frac{\sigma}{\sqrt{n}}$, where $n = 10$).

patterns, in the case of PTM dataset BioBERT *appears to heavily rely on surface patterns* reflected in our handcrafted distance-based patterns. The strong correlation between the surrogate model and the BioBERT-based model prediction points to the reliance of the model on such surface patterns, which will undoubtedly hinder the model's generalizability to external datasets. Therefore, before concluding OOD as a potential cause of generalization failure, we need to ensure that spurious correlations are NOT the source of a model's high performance. There are cases where some surface patterns might be reasonable for some tasks, we discuss such cases in detail in Section 4.3.

Detecting spurious correlations is non-trivial, while simple surrogate models can detect dominant surface patterns provided we know what to look for apriori. This approach has two main challenges: **a)** requires handcrafted features, and **b)** assumes that only a few dominant patterns exist. Deep learning models, such as transformers, that can potentially learn thousands of low frequency surface patterns (and these patterns may not be detectable by simple models), while these patterns may also be present in the test set resulting in inflated test performance.

3 Foundations of generalizability

The core idea behind generalizability is that the conclusions drawn, or a model inferred, from a sample can be applied to a wider population. In this section, we discuss some of the foundations of generalizability from clinical studies and why generalization failure cannot be solely attributed to out-of-distribution factors. Identifying the cause of generalization failures requires several components to be well-defined ahead of the experiments, which

are discussed in detail in this section.

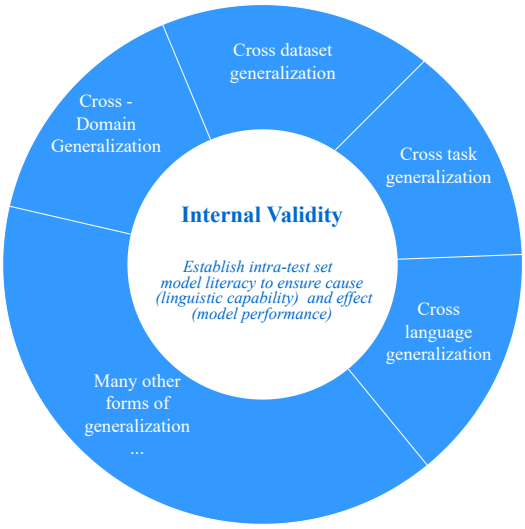

Figure 1: Internal validity is a mandatory precursor for any form of external generalization, including cross dataset generalization. Internal validity is required to ensure that the model has learned core linguistic strategies to solve the task within the context of the test set.

3.1 The notion of generalizability

Clinical studies aim to answer questions such as *"is this drug treatment effective?"*, and critically rely on generalizability to establish meaningful evidence (Rothwell, 2005; Guyatt et al., 2011b; Schünemann et al., 2013). A core element of a clinical study is the specification of the study population, referring to a subset of the population selected for research; it is impossible to study the entire population (Kukull and Ganguli, 2012). The implicit assumption is that conclusions drawn from the sample are applicable to the population, requiring the population boundary to be defined. This boundary depends on the aim of the study, can include various factors, including country, insurance memberships or disease status (Kukull and Ganguli, 2012). For instance, for a study that investigates the effects of a drug on a disease, the relevant population would typically be all the people with that disease. To ensure that any conclusions from the study using the samples drawn from the population are confidently generalizable to the entire relevant population, *intrinsic* and *extrinsic validity* of experiments (Guyatt et al., 2011a) must be established. We detail these concepts below.

3.2 Study Aim

In machine learning or more specifically NLP, the aim of a study might seem obvious, for example, to establish whether one model is better than the other for a given task according to a chosen metric. However, to be able to comprehensively answer the seemingly simple question, *"Is one model better than the other for a given task"*, can be a challenge. If the problem statement is well constrained, e.g. referring to performance on a benchmark such as GLUE (Wang et al., 2018), then the objective is clear. In real-world settings, the objective is usually to know if the model can meet certain performance objectives, e.g. will the model's predictions be at least 70% accurate when deployed. As a consequence, it becomes pertinent to define the population boundary or the context to ensure that the model performance is optimal for the task it is designed for in that broader context. Hence, defining the aim of the study requires careful definition of the target population.

3.3 Defining populations

In the context of machine learning, if a test set is a sample that effectively represents a population, then the conclusions based on the test set should apply to the entire population. For instance, if the conclusion is that the model has an accuracy of 90% based on the test set, it should mean that when the model is applied to the entire population, the prediction accuracy ideally should also be $\sim$90%.

In NLP, for the datasets used to benchmark model performance, such as GLUE (Wang et al., 2018), the broader "population" corresponding to these datasets is not clearly defined, and hence it is difficult to define the boundary or context of generalizability, *i.e.* the population that these results are meant to apply to or when data is out-of-distribution (OOD). As a result, when a model performs poorly on a different test set, an explanation that the data is OOD is insufficient unless the notion of distribution is clearly defined. We cannot simply attribute poor performance to OOD data. Model performance actually depends on **(a)** what the model has learned, and **(b)** how effective a test set is in measuring its performance. Moreover, OOD data should ideally have lower model confidence scores (Hendrycks and Gimpel, 2017). Thus, claims of OOD as an explanation for poor performance at the very least require the context of population or distribution to be clearly defined.

When we define a new task, we implicitly define the population boundary for the task, such as through the use of data cards (Pushkarna et al., 2022). For instance, if our task is to analyze the sentiment of IMDB movie reviews, IMDB movie

reviews are the population of texts that this model applies to. However, defining the boundary of this population is not trivial. It may require additional constraints around language, written vs. spoken style, and more precise specification of the domain, such as -restaurant vs. movie reviews.

An effective, well-informed boundary should consider key factors that can impact the performance of a model in a real-world scenario and constrains the problem space so that the samples can be drawn from the population that the model is meant to serve. Hence, defining the population boundary is a mandatory precursor to collecting training and test data to ensure that the collected samples are representative of the population.

3.4 Internal validity

Internal validity is crucial to ensure that the *cause and effect* is not affected by unintended consequence as a result of spurious correlations or bias in the data (Delgado-Rodríguez and Llorca, 2004), this particularly affects what we can infer from a gain in model performance.

To understand *internal validity* adapted from clinical studies, consider a hypothetical example of a customer sentiment analysis text classification task. To collect data, we may randomly select 500 customer emails from organization A (org-A), and another 500 from organization B (org-B). Let's assume that org-A generally provides better customer service than org-B, and that the samples from org-A contain a signature marker, "FROM-ORG-A". Say that a deep learning model that requires no feature engineering has over 90% accuracy, while another simpler model based on carefully curated semantic features achieves a performance of 75%. The software code is well tested, and the researchers also perform statistical significance tests and conclude that the deep learning model is better than the simpler model. However, the deep learning model has, in fact, relied on the signature "FROM-ORG-A" as a key indicator for positive labels, while the simpler model relies on the presence of words such as "great", "mediocre" to differentiate between classes. Is the conclusion that the deep learning model is better than the simple model at customer sentiment analysis internally valid, let alone generalizable to the wider population? The same parallels can be drawn from the case study of the PTM dataset discussed above, where the model seems to have relied on spurious correlations. Hence, the performance on a test set need not indicate that the model has the **basic linguistic task level literacy** even within the limited scope of the test set, as depicted in Figure 1.

Internal validity of experiments can also be affected by factors such as sample selection and instrumentation (Wortman, 1983). Internal validity is to ensure that the study and the conclusions are valid within the context of the experiment, where the cause (model has learned the right aspects of the language) and effect (model's performance) is fairly evident. Experimental errors such as bugs in the code, issues with test/training split resulting in data leakage (Elangovan et al., 2021) are obvious examples of errors that invalidate results. The internal validity can also be affected by selection of participants in the study (Patino and Ferreira, 2018). The participants of a study in NLP can be construed as the data and any human annotators. Lack of careful consideration of details such as training or test sample size, sample selection criteria etc. can make the study lack internal validity.

Performance gains made by large language models can be misunderstood as natural language understanding (Bender et al., 2021), hence performance on its own is not sufficient to infer more in-depth understanding. Geirhos et al. (2020) also emphasize the need to differentiate the capability required to perform on a dataset and the underlying capabilities of a model. Robustness of experimental design, data selection criteria, well-tested code, careful train-test split, effective test sets, statistical analysis, etc. are core aspects of internal validity in NLP.

3.5 External validity

External validity, associated with *transportability* of the results from samples to the wider population, is a heavily debated topic even in clinical studies, whereas internal validity is much more established in clinical studies (Tipton, 2014; Yarkoni, 2022; Degtiar and Rose, 2023). If a study is not internally valid, then external validity is irrelevant (Patino and Ferreira, 2018). Assuming that study results are internally valid, whether the conclusions of a study are generalizable or transportable to the wider population beyond the examined datasets depends on the ability to separate "relevant" from "irrelevant" facts for the study. More importantly, well-designed population-based studies can minimize the risk of *selection factors with unintended consequences* on study results Kukull and Ganguli (2012).

Spurious correlations in training data affect internal validly as the model is set up to learn irrelevant facts, while training samples that do not sufficiently represent the underlying population affect external validity (Delgado-Rodríguez and Llorca, 2004). In clinical studies, conclusions drawn from the sample may lack external validity when there are differences between study samples and the target populations, such as subject characteristics or hospital procedures (Degtiar and Rose, 2023). For an equivalent example in NLP, consider sentiment analysis. A trained model with a set of words such as "good" associated with positive sentiment may be internally valid, but may fail to perform well on the wider population when it encounters newer terms such as "heartwarming".

In NLP, even though there is no single comprehensive formal definition of OOD (Arora et al., 2021), conceptually generalization challenges stemming from OOD can generally be considered external validity challenges. OOD can be a result of domain or distribution shift, due to languages or tasks differing from training data (Hupkes et al., 2023), or even samples from adversarial attacks (Omar et al., 2022).

4 Discussion

4.1 Is the generalization failure due to internal or external validity?

Attributing the right cause of failures enables us to take the most effective corrective action, hence separating internal vs. external factors is important, given internal factors are far more controllable than external ones. Ensuring internal validity requires that we understand cause and effect of a model's performance. This in turn forces researchers to analyze the data, investigate training methods that are robust against issues in the training data such as noisy labels and spurious correlations. High performance on the test set is clearly not sufficient to ensure that the model is capable of solving the task it is trained for, as similar spurious correlations can exist in both training and test sets. Training data is rarely perfect, as they can contain many problems from annotator bias (Gururangan et al., 2018), incorrect or noisy labels to spurious correlations (McCoy et al., 2019; Gururangan et al., 2018). Hence, ensuring internal validity at the very least requires the following checks:

1. How many spurious correlations or noisy labels are present in training and/or test data?
2. How diverse is the training data, and is it sufficient in volume to learn the right features for a given task?
3. How robust is the training procedure against spurious correlations or noisy labels?
4. Were model explainability analyses able to identify the model's reliance on spurious correlations?
5. Are experiments well-designed and reproducible?
6. How effective is the test set in verifying what the model has learned and/or weaknesses in the model?

Questions 1-4 can be difficult to answer accurately in practice due to deficiencies in the current set of tools and technologies available to analyze the large volumes of data for surface patterns. They may rely on domain knowledge. It may simply be expensive to collect more training data. These challenges are compounded by the fact that neural networks are difficult to understand.

Good test sets, on the other hand, provide a pragmatic way to understand the capabilities of a model, even without access to the underlying model architecture. Ideally, the size of the randomly sampled test set should be sufficiently large, as a large sample size is much more likely to representative of true performance than a smaller one (Faber and Fonseca, 2014). Ribeiro et al. (2020) use the principles of software testing to test models, essentially behavioral testing the models using a *CheckList* of test cases. The *CheckList* tests the model against a set of linguistic capabilities such as negation, replacing named entities etc. This requires careful curation of test examples and requires that these samples are updated as the capabilities of the model improve. Similar strategies have been employed to develop test suites for concept recognition systems (Cohen et al., 2010; Groza and Verspoor, 2014) and negation inference (Truong et al., 2022). Kiela et al. (2021) develop Dynabench to continuously update the test set samples with human-in-the-loop.

4.2 Establishing cause and effect in models

In clinical studies, randomized control trials (RCT) form the gold standard of evidence to establish *cause and effect* of treatment or interventions (Hariton and Locascio, 2018) and their outcomes. In a RCT, participants of the study are randomly assigned to a "experimental" and "control" group,

where the experimental group receives the intervention and the control group receives a placebo (Kendall, 2003). The key intuition is that if the only non-random difference between the experimental and control group is the intervention, then the intervention must be the cause of the outcome of the intervention.

Adapting this approach to NLP benchmarks could help ensure that that models are assessed for their linguistic capabilities. One pragmatic option to doing this may be to curate a counterpart 'control' test set for the standard randomly sampled test set. The control test set would be created by making minor perturbations to a sample in the original test set such that the ground truth label is altered, e.g. through the use of contrast sets Gardner et al. (2020). The idea here is that if the model has effectively learned the key linguistic aspects required to predict a given label, then the model should change its prediction when given a perturbed instance. Furthermore, we suggest that a model's prediction should be marked as correct if and only if its prediction on a perturbed counterpart is also correct. This would ensure that the model is judged for its linguistic skills at least within the context of the test set, ensuring internal validity.

4.3 How unreliable is a surface pattern?

While it may be impossible to prevent models from relying on surface patterns, we specifically need to watch out for model's dependence on spurious correlations or features that tend to be highly unreliable, e.g. the distance between the participating entities in relation extraction discussed above.

Generalizability of deep learning networks depends on whether they learn **(a)** spurious correlations, **(b)** reasonable heuristics, or **(c)** oracle true language meaning. Oracle true meaning refers to true language understanding that takes into account the meanings of the individual words as well as the interplay between them relevant to produce the output of a target task. Spurious correlations are surface patterns with little or no linguistic backing whereas heuristics are plausible surface patterns that may generally work without the need for deeper comprehension, and thus generalizability is adversely impacted by spurious correlations, making the model internally invalid. For instance, a model that associates the presence of the word "good" in a review with a positive sentiment has captured a heuristic; it is a reasonable rule but may not produce a correct prediction when used in the context of contradiction or sarcasm. Spurious correlations can render the model useless beyond the test set.

5 Related works

5.1 Spurious correlations

There are several reports of spurious correlations in NLP models and benchmark datasets. In the MNLI dataset (Williams et al., 2018), McCoy et al. (2019) find that BERT relies on lexical overlap between hypothesis and premise. In the SNLI dataset (Bowman et al., 2015), Gururangan et al. (2018) find that negation words such "no", "never" are indicators of contradiction in the NLI task, while sentence length of the neutral hypotheses tends to be long. In the SQUAD dataset (Rajpurkar et al., 2016) for Question Answering (QA), Shinoda et al. (2022) find that the relation position of the answer can be used as surface patterns by the QA models. Approaches to detect spurious features without apriori handcrafting them have also been studied, e.g. Utama et al. (2020), relying on the observation that pre-trained models exploit simple patterns in the early stage of the training phase. Training a model to be robust against spurious correlations is also an active area of research, e.g. Tu et al. (2020) find that multitask learning improves generalization. Data-driven approaches such as the use of h-adversarial training samples (Elangovan et al., 2023) can also improve generalization.

6 Conclusion

Generalization of machine learning models in NLP is a complex topic. Clinical research offers guiding principles on how to understand generalization, including precise population definitions and contrasting controls. There are various points of failure in NLP modelling that can produce results that may not be generalizable. Out-of-distribution (OOD) effects may be an overly simplistic explanation for generalization failures. Attributing causation to generalization failures requires detailed investigation into some potential pitfalls affecting internal validity. Ensuring internal validity requires at least an effective test set that controls for spurious correlations in the training data. More careful construction of evaluation frameworks will ensure appropriate inferences about the relationship between *cause* (model's linguistic capabilities) and *effect* (performance) from experimental results.

Limitations

Internal validity can be compromised for various reasons, broadly speaking, data vs non-data related problems. Non data related issues can be bugs in code. Data related problems such label noise, poor quality annotation can also make a model internally invalid. In this paper, we have primarily focused on spurious correlations, assuming that the labels themselves are of high quality.

As mentioned in section 2.4, identifying spurious correlations that a model relies on is non-trivial. A simple surrogate model used in our case study can only detect the dominant spurious features, while a deep learning model such as BERT can learn thousands of such spurious features. Hence, if the simple surrogate model has poor performance, it does not mean that the model has not relied on spurious features.

Ethics Statement

This work does not involve collection of new data; all analysis relies on previously published data sets. Our work adheres to the ACL Ethics Policy[1].

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A Appendix: PTM-PPI dataset Decision-tree

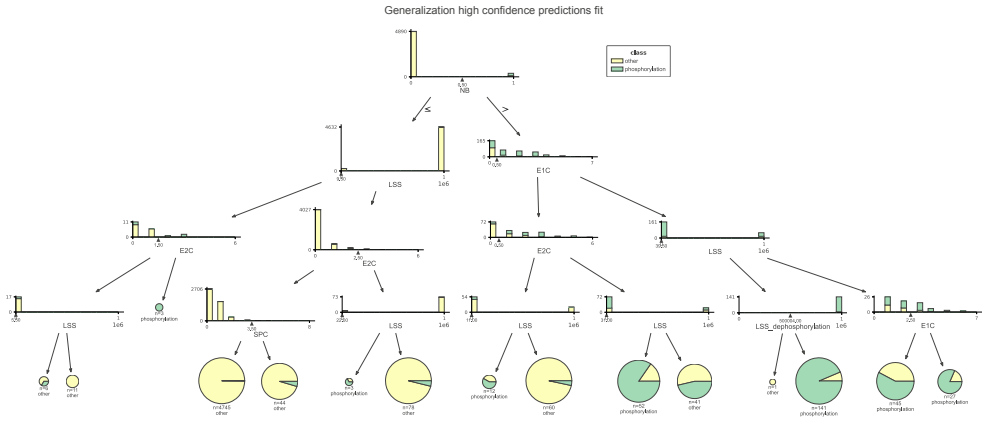

Figure 2: Decision Tree (NB-T) fit in high confidence predictions in the generalization set

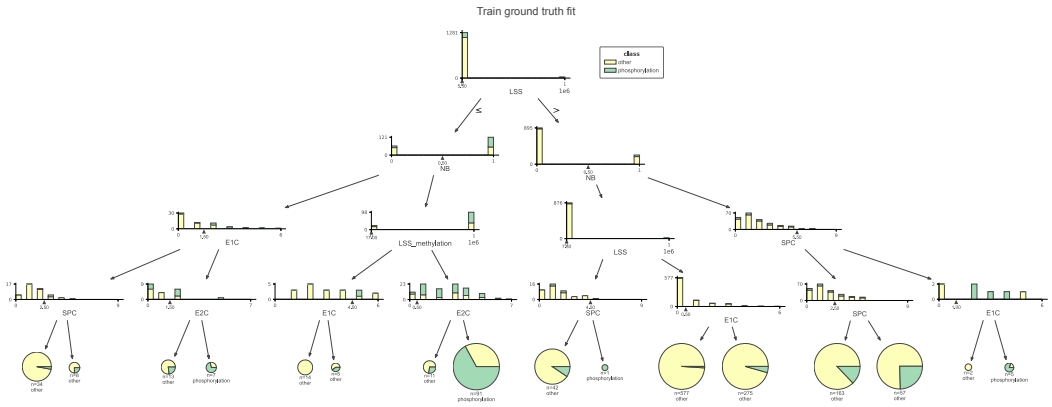

Figure 3: Decision Tree (NB-T) fit in Train ground truth fit

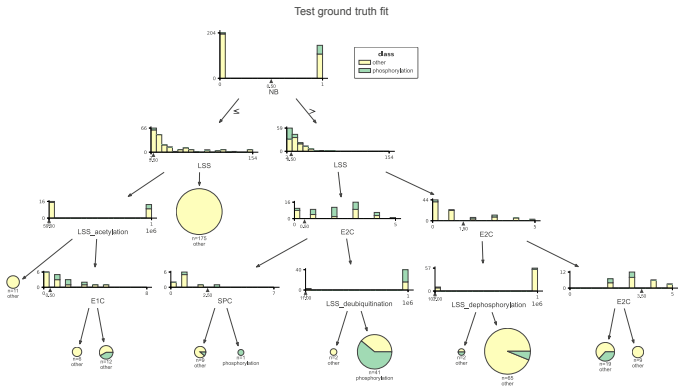

Figure 4: Decision Tree (NB-T) fit in Test ground truth fit

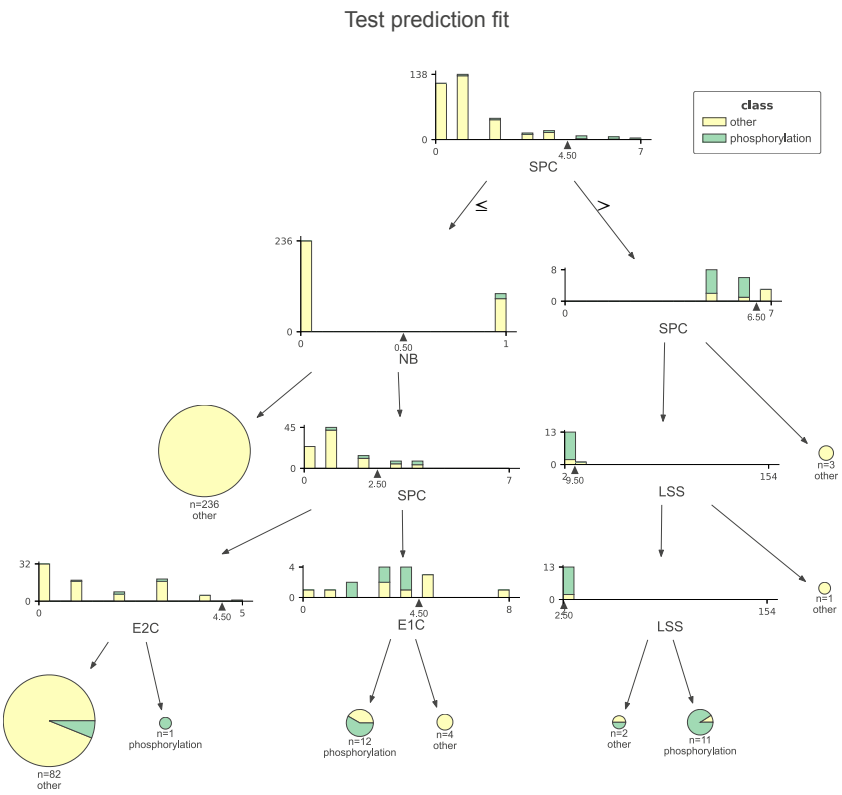

Figure 5: Decision Tree (NB-T) fit in Test set BioBERT predictions fit