Bayesian Concept Bottleneck Models with LLM Priors

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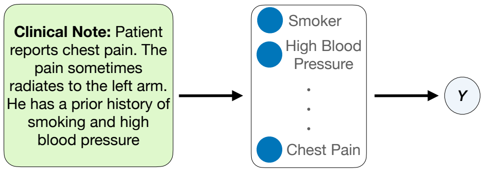
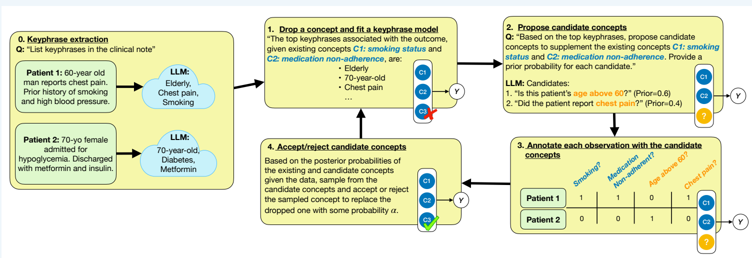


Motivation

- Concept Bottleneck Models (CBMs) leverage black-box models to extract interpretable concepts, which serve as inputs to a transparent prediction model.
- CBMs currently require human experts to identify and extract a set of candidate concepts a priori. The size of this set is limited by practical constraints and, more importantly, may not include truly relevant concepts.

BC-LLM

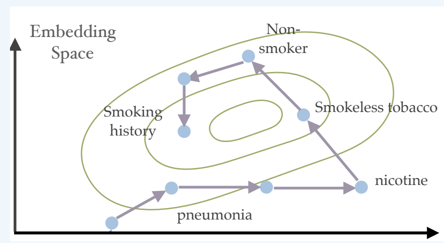
- Leverage LLMs to provide a prior over concepts, propose candidate concepts, extract concepts, and iteratively refine the concepts.
- To overcome errors or inconsistencies in the LLM, BC-LLM frames the LLM-guided concept search as a Bayesian posterior sampling procedure, which allows for statistically rigorous inference and uncertainty quantification:
  - ***Theorem (Informal):*** *Even if the LLM defines an imperfect prior, BC-LLM will converge to the true concepts asymptotically.*



Overview of BC-LLM

Efficient LLM Search over Concepts

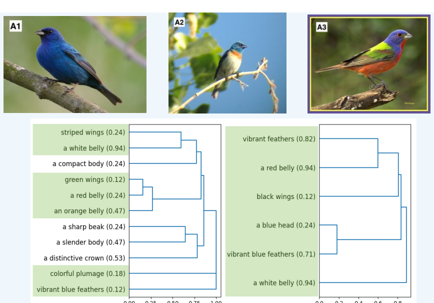
- Formally, BC-LLM searches over candidate concepts using *Gibbs sampling*.
- To search over concepts as efficiently as possible, we leverage *Multiple Try Split-Sample Metropolis-within Gibbs*, *in which* the LLM proposes multiple candidate concepts each iteration and selects the one best aligned with the data.



Example sampling procedure for a single concept

BC-LLM learns accurate yet interpretable concept bottleneck models by using LLMs to iteratively hypothesize, annotate, and refine candidate concepts within a statistically rigorous Bayesian framework

Paper



Left and right dendrograms are concepts learned using 1/3 versus all of the training data. Highlighted concepts are distinguishing bird features.

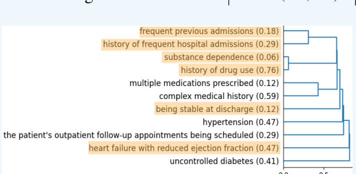
Experiment: Bird type classification

- Task: Learn a CBM to predict bird type. To make the task more difficult and prevent test data leakage, the LLM is not told it is classifying bird types.
- BC-LLM outperforms all other CBM learning procedures and performs as well as, if not better, than black-box models.

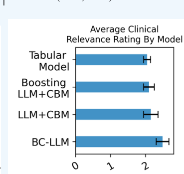
AUCs of CBMs and black box (ResNet) for classifying bird subcategories

	In-distribution			*OOD*
Method	Accuracy (↑)	AUC (↑)	Brier (↓)	Entropy (↑)
BC-LLM	**0.680** (0.614, 0.747)	**0.874** (0.840, 0.907)	**0.428** (0.357, 0.500)	0.865 (0.693, 1.036)
LLM+CBM	0.640 (0.573, 0.707)	0.810 (0.768, 0.853)	0.452 (0.377, 0.528)	0.663 (0.474, 0.852)
Boosting LLM+CBM	0.538 (0.463, 0.614)	0.722 (0.673, 0.772)	0.577 (0.499, 0.654)	0.842 (0.630, 1.054)
Human+CBM	0.658 (0.591, 0.725)	0.835 (0.791, 0.879)	0.499 (0.414, 0.584)	0.758 (0.558, 0.959)
LLM+CBM (No keyphrases)	0.555 (0.488, 0.623)	0.759 (0.713, 0.805)	0.651 (0.548, 0.754)	0.626 (0.495, 0.757)
ResNet	0.664 (0.613, 0.716)	0.853 (0.821, 0.885)	0.457 (0.398, 0.516)	**0.914** (0.748, 1.079)

Method	AUC (95% CI)	Brier (95% CI)
BC-LLM	**0.64** (0.58, 0.70)	**0.14** (0.12, 0.62)
LLM+CBM	0.59 (0.52, 0.65)	0.29 (0.25, 0.33)
Boosting LLM+CBM	0.59 (0.52, 0.66)	**0.14** (0.12, 0.16)
Bag-of-words	0.52 (0.46, 0.58)	0.29 (0.25, 0.34)



Concepts learned by BC-LLM where highlighted concepts received scores from clinicians as being highly predictive



Average clinical ratings for concepts from different methods

Experiment: Revising a Readmission Risk Prediction Model with Clinical Notes

- Task: Determine if there are useful concepts in discharge notes for improving on an existing tabular model for predicting 30-day unplanned readmission risk. Learn a CBM that revises the existing risk prediction by extracting 4 concepts from clinical notes.
- BC-LLM outperforms all other CBM learning procedures.
- Survey results: Clinicians found the BC-LLM model to be
  - More clinically meaningful and interpretable
  - Contained more causally relevant features
  - More actionable, i.e. suggested clinical actions for reducing readmission risk