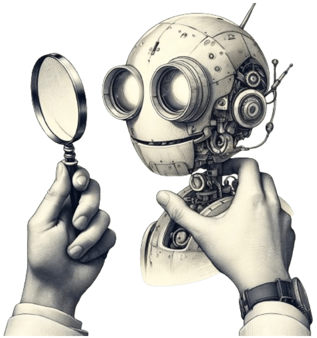
Foundations of Interpretable AI

Tutorial @ CVPR Nashville JUNE 11-15, 2025



PART I: Motivation and Post-hoc Methods (9:00 – 9:45 am) Aditya Chattopadhyay (Amazon)

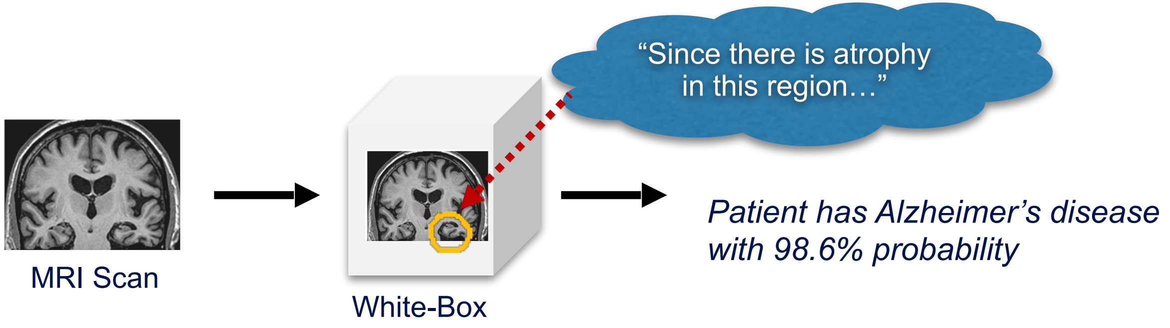
PART II: Shapley Value Based Methods (9:45 – 10:30 am) Jeremias Sulam (Johns Hopkins)

☕ Coffee break ☕ (10:30 – 11 am)

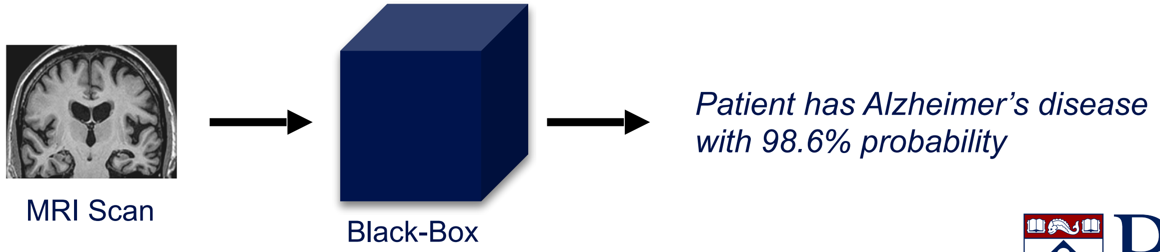
PART III: Interpretable by Design Methods (11 – 11:45 am) René Vidal (Penn)

Interpretability Crisis

- As deep learning is widely used in safety critical applications, there is a need for developing trustworthy and interpretable models.
- Ideally we desire...

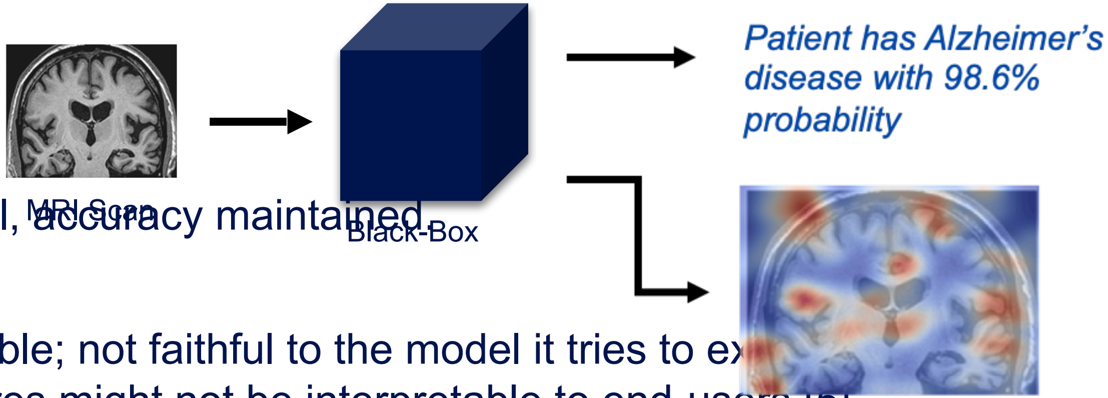


- But in reality



Main Trend: Post-hoc Explanations

- Most method interpret black-box models post-hoc using importance scores based on the sensitivity of the model output to the input features:
  - LIME [1]
  - Grad-CAM [2]
  - SHAP [3]



- **The Good**:
  - No need to retrain model, accuracy maintained.
- **The Bad**:
  - Explanations are unreliable; not faithful to the model it tries to ex
  - Feature importance scores might not be interpretable to end-users [5].

[1] Ribeiro, Singh, Guestrin. "Why Should I Trust You?" Explaining the Predictions of Any Classifier. KDD, 2016.
[2] Selvaraju, Cogswell, Das, Vedantam, Parikh, Batra. Grad-CAM: Visual Explanations from Deep Networks via Gradient-based Localization. ICCV 2017.
[3] Lundberg and Su-In Lee. A Unified Approach to Interpreting Model Predictions. NIPS, pp 4765–4774, 2017.
[4] Adebayo, J., Gilmer, J., Muelly, M., Goodfellow, I., Hardt, M., & Kim, B. Sanity checks for saliency maps. NeurIPS, 2018
[5] Rudin. Stop explaining black box machine learning models for high stakes decisions and use interpretable models instead. Nature Machine Intelligence, 2019.

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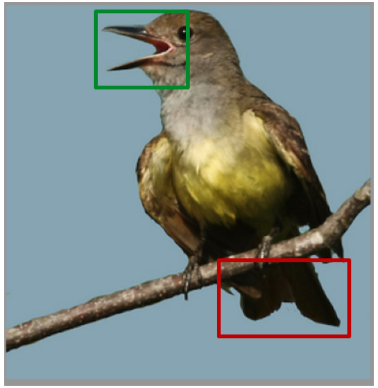
Need for Interpretable-by-Design Models

- Explanations are user/task/domain dependent and best described in terms of words/attributes/facts that support the decision's reasoning.
- We can capture this via a user/task/domain dependent query set Q.

(a) **Task**: bird classification
Queries: parts, attributes



(b) **Task**: scene interpretation
Queries: objects, relationships

(c) **Task**: medical diagnosis
Queries: symptoms

0. Ear pain
1. Sore throat
2. Fever
3. Cough
4. Nasal congestion
5. Allergic reaction
6. Shortness of breath
7. Painful sinuses

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Concept Bottleneck Models (CMBs)

- Concept Bottleneck Models (CBMs) [1].
  - Specify a query set: define a set of task-relevant concepts Q.
  - Answer queries: train deep network to predict concepts from Q in image x.
  - Make prediction: train linear classifier on predicted concepts.
- Explain prediction via weights of linear layer for different concepts.

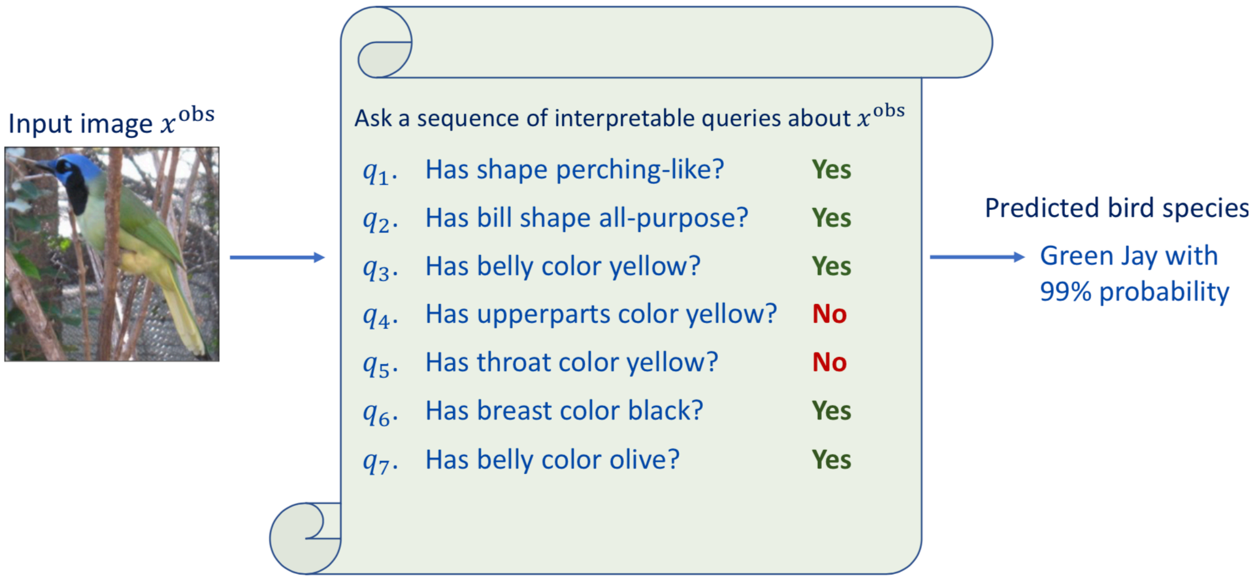
[1] Koh, P. W., Nguyen, T., Tang, Y. S., Mussmann, S., Pierson, E., Kim, B., & Liang, P. Concept bottleneck models. ICML, 2020.

Are Concept Bottleneck Models Enough?

- Limited expressivity: linear classification layer limits expressivity of CBMs when "concept answers → class prediction" map is non-linear.
- Limited interpretability: explanations in terms of coefficients of linear weights not always desirable to end-users, especially non-AI experts.
- Limited flexibility: same explanations for all inputs in the same class.

Information Pursuit Framework

- **Information Pursuit**: interpretable-by-design framework based on:
  - Selecting the smallest number of queries that are sufficient for prediction.
  - Making a prediction based only on the chain of query-answer pairs.



[1] Chattopadhyay, Slocum, Haeffele, Vidal, Geman. Interpretable by design: Learning predictors by composing interpretable queries. *TPAMI 2022.*

Ingredients Needed to Implement this Framework

- **Q1: How do we define the set of queries?**
  - Defined by domain experts [1]

- **Q2: Given an input and a query, how do we answer the query?**
  - Train classifiers on data annotated with query answers by task experts [1].

-
  - **Information Pursuit**: Select smallest number of queries that are sufficient

[1] Chattopadhyay, Slocum, Haeffele, Vidal, Geman. Interpretable by design: Learning predictors by composing interpretable queries. TPAMI 2022.
[2] Chattopadhyay, Chan, Haeffele, Geman, Vidal. Variational Information Pursuit for Interpretable Predictions, ICLR 2023.
[3] Chattopadhyay, Pilgrim, Vidal. Information Maximization Perspective of Orthogonal Matching Pursuit with Applications to Explainable AI. NeurIPS 2023.
[4] Chattopadhyay, Chan, Vidal. Bootstrapping Variational Information Pursuit with Foundation Models for Interpretable Image Classification. ICLR 2024.
[5] Chattopadhyay, Haeffele, Vidal, Geman. Performance Bounds for Active Binary Testing with Information Maximization. ICML 2024.

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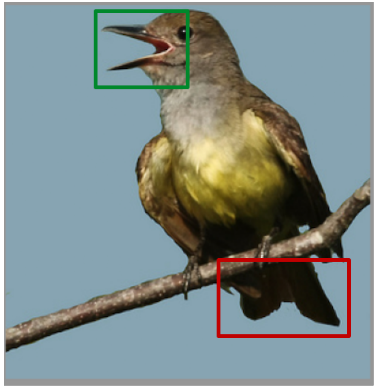
Q1: How to define the set of queries?

Q1: How do we Define the Set of Queries?

- Defined by domain experts [1,2]
  - Assume queries have similar semantic resolution.
  - **CUB dataset**
    - 200+ bird classes
    - 300+ bird attributes
  - **SymCAT-200 dataset**
    - 200 disease diagnosis
    - 326 patient symptoms
  - **Challenge**
    - Annotating queries is very costly

(a) **Task**: bird classification
Queries: parts, attributes



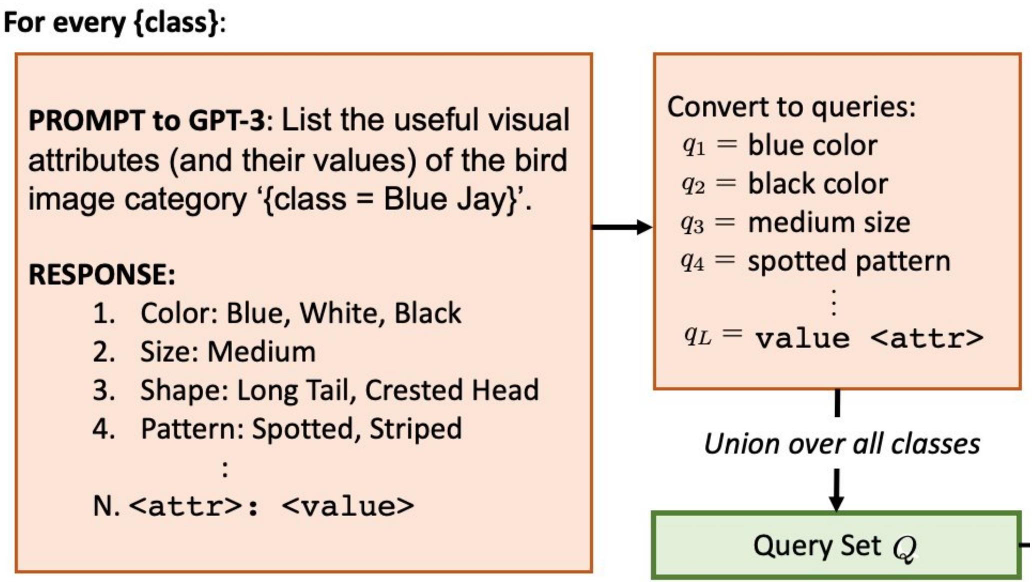
(c) **Task**: medical diagnosis
Queries: symptoms

0. Ear pain
1. Sore throat
2. Fever
3. Cough
4. Nasal congestion
5. Allergic reaction
6. Shortness of breath
7. Painful sinuses

[1] Koh, P. W., Nguyen, T., Tang, Y. S., Mussmann, S., Pierson, E., Kim, B., & Liang, P. Concept bottleneck models. ICML, 2020.
[2] Chattopadhyay, Slocum, Haeffele, Vidal, Geman. Interpretable by design: Learning predictors by composing interpretable queries. TPAMI 2022.
[3] Oikarinen, T., Das, S., Nguyen, L. M., & Weng, T. W. (2023). Label-free concept bottleneck models. ICLR 2023
[4] Chattopadhyay, Chan, Vidal. Bootstrapping Variational Information Pursuit with Foundation Models for Interpretable Image Classification. ICLR 2024.

Q1: How do we Define the Set of Queries?

- Defined by large language models [3,4].
  - E.g., ask LLM for list of attributes of all relevant categories.



[1] Koh, P. W., Nguyen, T., Tang, Y. S., Mussmann, S., Pierson, E., Kim, B., & Liang, P. Concept bottleneck models. ICML, 2020.
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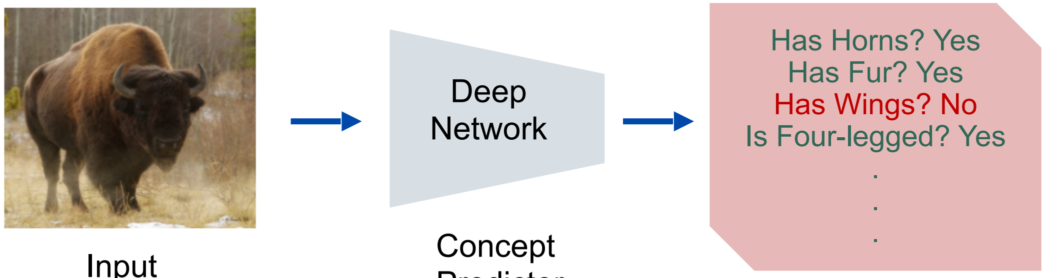
[4] Chattopadhyay, Chan, Vidal. Bootstrapping Variational Information Pursuit with Foundation Models for Interpretable Image Classification. ICLR 2024.

Q2: Given an input and a query, how do we answer the query?

Q2: How do we Answer a Query for a given Input?

- Train classifiers on data annotated with query answers [1].



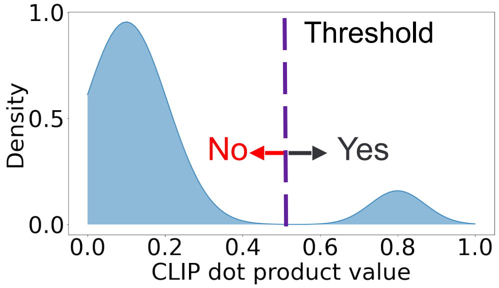
  - **Challenge:** need tons of data annotated with all concepts/attributes/facts => few datasets have such detailed annotations.
  - **Challenge:** cannot handle new queries that have not been annotated.

[1] Koh, P. W., Nguyen, T., Tang, Y. S., Mussmann, S., Pierson, E., Kim, B., & Liang, P. Concept bottleneck models. ICML, 2020.

Q2: How do we Answer a Query for a given Input?

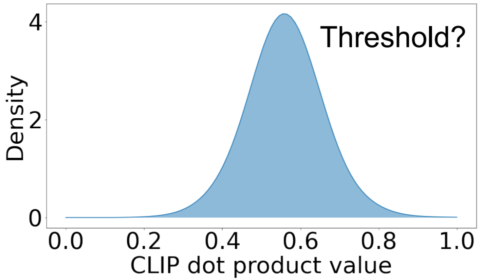
- Use Vision Language Models (VLMs) to answer queries
  - **Challenge:** State-of-the-art VLMs like Llama [1] and BLIP [2] are too slow to be used in an online manner.
  - **Challenge**: CLIP [3] is relatively light-weight, but CLIP dot products between query and image are inadequate: they are not interpretable.

<u>Desired</u> distribution of CLIP dot products



Input image x^{obs}

<u>Observed</u> distribution of CLIP dot products



[1] Touvron, Lavril, Izacard, Martinet, Lachaux, Lacroix, Rozière et al. "Llama: Open and efficient foundation language models." arXiv preprint arXiv:2302.13971, 2023.
[2] Li, Junnan, et al. "Blip-2: Bootstrapping language-image pre-training with frozen image encoders and large language models." ICML 2023.
[3] Radford, Kim, Hallacy, Ramesh, Goh, Agarwal, Sastry et al. "Learning transferable visual models from natural language supervision." ICML 2021

Q2: Can we Improve CLIP without Annotations?

- In image classification, most query answers are known to be false based on the class alone.
  - **Example**: Know class is dog → "does the subject have fins?" is false → no need to see the image.

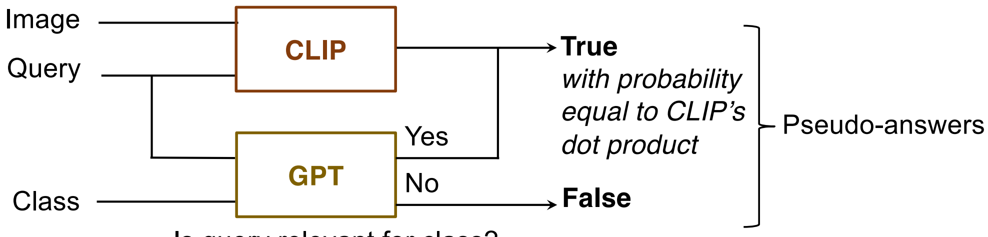
Yes! Use LLMs

Input image x^{obs}

- We need to look at the image only for queries relevant to the class.
  - **Example**: "Does the subject have a leash?". Need to see image since not all dogs have a leash.

Concept Question Answering System [1]

- **Pseudo-labeling**: Use GPT to determine class-relevant queries and use CLIP to determine probability of being true based on image.

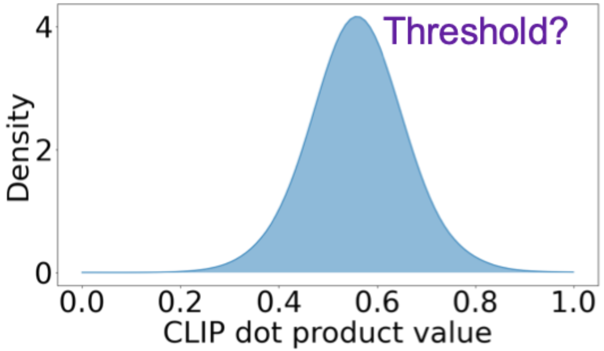


- **Concept-QA**: Train a lightweight visual question answering (VQA) system using pseudo-answers as we don't know class at test time.

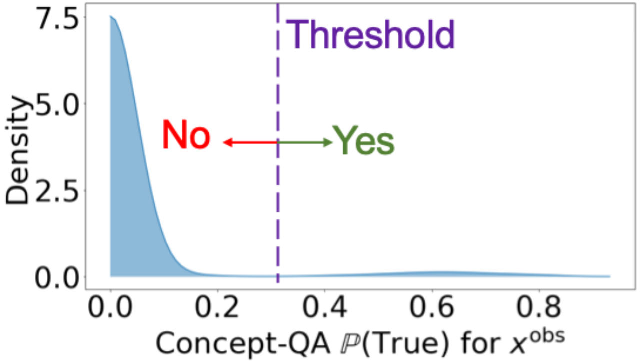
[1] Chattopadhyay, Chan, Vidal. "Bootstrapping Variational Information Pursuit with Foundation Models for Interpretable Image Classification." ICLR 2024

Interpretability of Concept-QA answers

- Concept-QA is more interpretable than CLIP!



Input image x^{obs}



Accuracy of Concept-QA answers

- Concept-QA is more accurate than CLIP & more efficient than BLIP2:
  - Concept-QA takes 0.04s per query vs 1.52s per query for BLIP2 FlanT5 model!

Model	ImageNet		Places365		CUB-200		CIFAR-10		CIFAR-100	
	Acc.	F_1	Acc.	F_1	Acc.	F_1	Acc.	F_1	Acc.	F_1
CLIP-Bin_{std}	0.55	0.39	0.58	0.42	0.56	0.48	0.58	0.47	0.51	0.21
CLIP-Bin_{norm}	0.50	0.27	0.49	0.26	0.56	0.45	0.66	0.53	0.54	0.24
BLIP2 ViT-g $\text{OPT}_{2.7\text{B}}$	0.55	0.31	0.76	0.18	0.53	0.35	0.73	0.13	0.86	0.07
BLIP2 ViT-g $\text{FlanT5}_{\text{XL}}$	0.86	**0.56**	**0.87**	**0.62**	0.70	0.40	**0.83**	0.59	**0.87**	**0.41**
Concept-QA (Ours)	**0.87**	**0.56**	0.83	0.45	**0.80**	**0.54**	0.80	**0.62**	0.80	0.38

Manually annotated 2.5K randomly sampled image-query pairs for each dataset.

Q3: How do we select the queries that form an explanation?

Information Pursuit (IP)

- **Q3: How do we select queries that form the explanation?**
  – Shorter chains are easier to interpret.
  – Select smallest number of queries that are sufficient for prediction.

Generative-IP (G-IP) [1]

Learn deep generative model and use it to select most informative queries.

Variational-IP (V-IP) [2]

Train deep network to select the next optimal query given answers thus far.

IP-OMP [3]

Use orthogonal matching pursuit and large vision and language models.

[1] Chattopadhyay, Slocum, Haeffele, Vidal, Geman. Interpretable by design: Learning predictors by composing interpretable queries. TPAMI 2022.
[2] Chattopadhyay, Chan, Haeffele, Geman, Vidal. Variational Information Pursuit for Interpretable Predictions, ICLR 2023.
[3] Chattopadhyay, Pilgrim, Vidal. Information Maximization Perspective of Orthogonal Matching Pursuit with Applications to Explainable AI. NeurIPS 2023.
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[5] Chattopadhyay, Haeffele, Vidal, Geman. Performance Bounds for Active Binary Testing with Information Maximization. ICML 2024.

Information Pursuit: Problem Formulation

- Notation
  - $X \in \mathscr{X}$: input variable (data).
  - $Y \in \mathscr{Y}$: prediction variable (label).
  - $Q = \{q : \mathscr{X} \to \mathscr{A}\}$: query set.

$$X \xrightarrow{\quad} \boxed{q} \xrightarrow{\quad} a$$

- Querier π : a function that selects the next question given history.

$$(q_{1:k}, \ a_{1:k}) \xrightarrow{\quad} \boxed{\pi} \xrightarrow{\quad} q_{k+1}$$

- $\mathrm{Code}^{\pi}_{Q}(X)$: chain of query-answers selected by the querier for input X.

$$(q_{1:k}, \ a_{1:k})$$

Information Pursuit: Optimal Querier

- What properties should an ideal querier have?
  - Minimality: shorter explanations are easier to interpret and thus preferred.
  - Sufficiency: explanations (query-answer chains) should be a sufficient statistic for Y.

- Balance minimality of explanation with sufficiency via the objective:

$$\min_{\pi} \mathbb{E}\left[\left|\mathrm{Code}_Q^{\pi}(X)\right|\right] \qquad \text{(Minimality)}$$

$$\text{s.t.} \quad \mathbb{P}\left(Y \middle| \mathrm{Code}_Q^{\pi}(X)\right) = \mathbb{P}(Y \mid X) \qquad \text{(Sufficiency)}$$

- Above problem is NP-Hard to solve [1], thus need for approximations.

[1] H. Laurent and R. L. Rivest, "Constructing optimal binary decision trees is np-complete", Inf. Process. Lett., vol. 5, no. 1, pp. 15-17, 1976.

Generative Information Pursuit (G-IP)

- Given query set Q, Information Pursuit (IP) selects queries sequentially and adaptively in order of information gain [1].

Information Pursuit Algorithm

Queries are chosen according to observed x.

- First query and prediction:

$$q_1 = \arg\max_{q \in Q} I(q(X); Y) \qquad y_1 = \arg\max_{y \in Y} \mathbb{P}(y \mid q_1(x))$$

- Next query and prediction:

$$q_{k+1} = \arg\max_{q \in Q} I(q(X); Y \mid q_{1:k}(x)) \qquad y_{k+1} = \arg\max_{y \in Y} \mathbb{P}(y \mid q_{1:k+1}(x))$$

- Termination and prediction:

$$q_{L+1} = q_{STOP} \quad \text{if} \quad \max_{q \in Q} I(q(X); Y \mid q_{1:L}(x)) = 0 \qquad y_{L+1} = \arg\max_{y \in Y} \mathbb{P}(y \mid q_{1:L}(x))$$

$q_{1:k}(x)$ is the event that contains all realizations of X that agree on the first k query-answers for x.

[1] Geman and Jedynak, An active testing model for tracking roads from satellite images, TPAMI, 1996.

Generative Information Pursuit (G-IP)

- Selecting the first query requires computing

$$\underset{q\in Q}{\operatorname{argmax}}\ I\big(q(X);Y\big)$$

History

- Later queries need computing

$$\underset{q\in Q}{\operatorname{argmax}}\ I\big(q(X);Y \mid q_{1:k}(x)\big)$$

- **Generative IP**: learn deep generative model for $\mathbb{P}(q(X);Y)$ and use it to compute mutual information (via sampling) and select best query.
- **Challenge**: estimating mutual information in high dimensions is hard.

[1] Chattopadhyay, Slocum, Haeffele, Vidal, Geman. (2022). Interpretable by design: Learning predictors by composing interpretable queries. TPAMI 2022.

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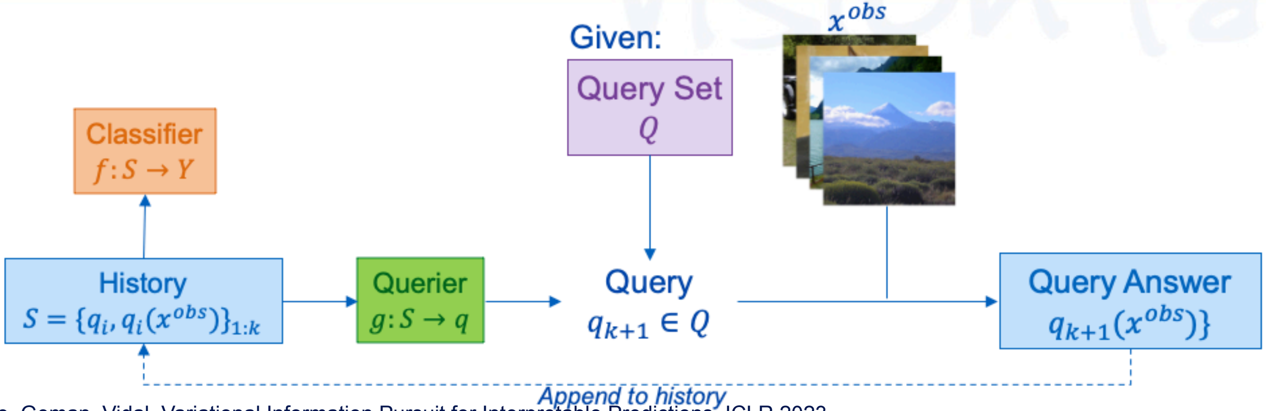
Variational Information Pursuit (V-IP)

- Train querier g_η to select the most informative query for classifier f_θ.

$$\min_{\theta,\eta} \mathbb{E}_{X,S}\left[D_{KL}\left(\mathbb{P}(Y \mid X) \,||\, \mathbb{P}_\theta\left(Y \mid q_\eta, S\right)\right)\right]$$

$$s.t. \quad q_\eta = g_\eta(S), \quad \mathbb{P}_\theta\left(Y \mid q_\eta, S\right) = f_\theta\left(q_\eta \cup S\right)$$

- **Theorem:** selecting the most informative query given history ≡ finding query that, when added to the history, gives best prediction.



[2] Chattopadhyay, Chan, Haeffele, Geman, Vidal. Variational Information Pursuit for Interpretable Predictions, ICLR 2023.

IP vs Orthogonal Matching Pursuit (OMP)

- **IP:** Given queries selected thus far, IP selects query that is most informative for Y

$$q_{k+1} = \underset{q \in Q}{\operatorname{argmax}}\ I\big(q(X); Y \,\big|\, q_{1:k}(x)\big)$$

- **OMP:** given atoms selected thus far, OMP selects atom that is most correlated with x

$$\min_{\beta}\ ||\beta||_0 \text{ s.t. } D\beta = x$$

$$i_{k+1} = \underset{d \in D}{\operatorname{argmax}}\ |\langle d,\ x - D\beta_k \rangle|$$

- **CLIP-IP-OMP [1]:** decompose image as sparse linear combination of semantic dictionary

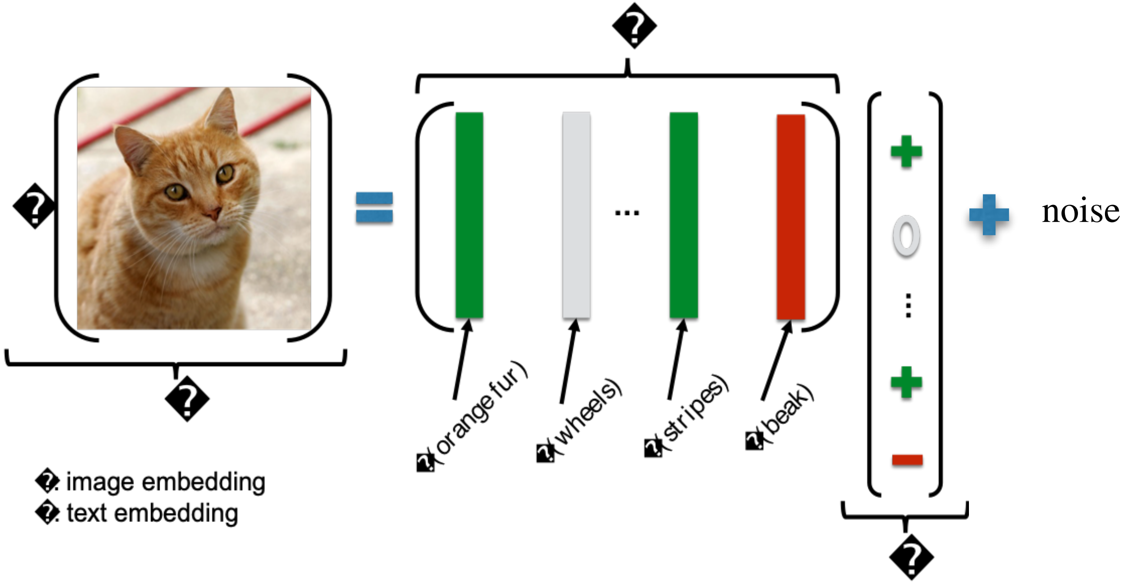
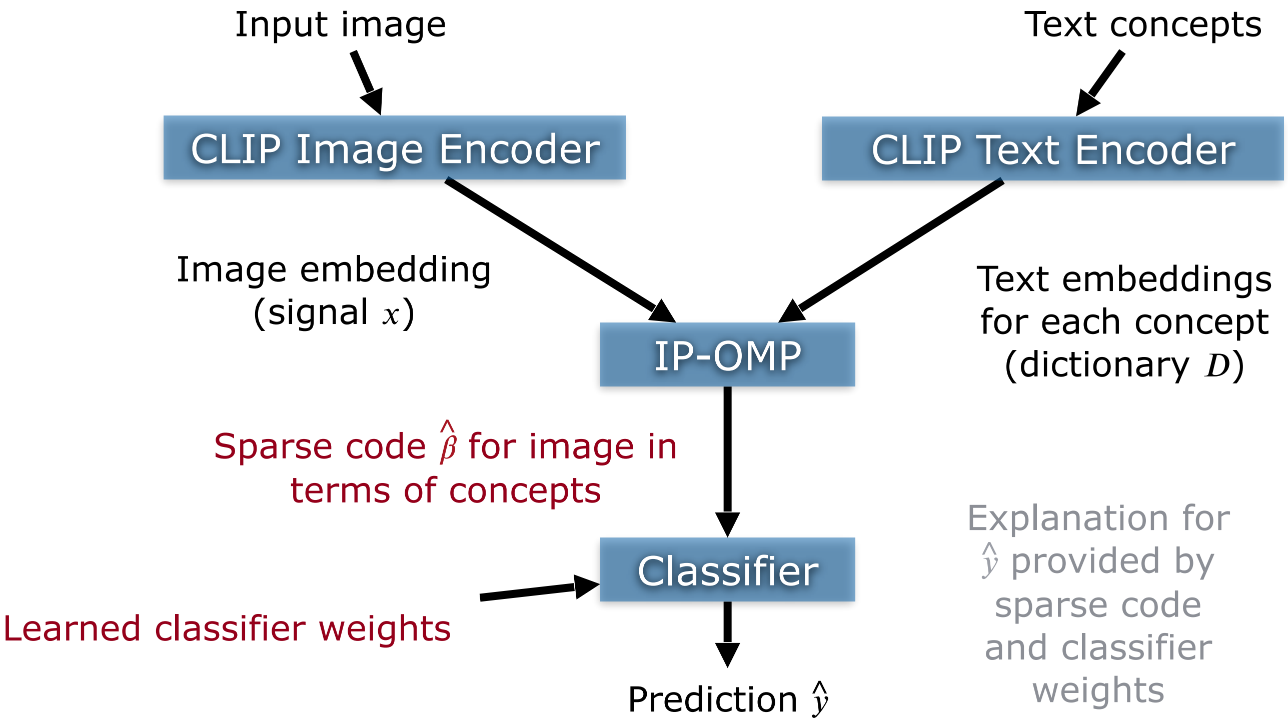


Image credit: https://en.wiktionary.org/wiki/cat#/media/File:Cat03.jpg

[1] Chattopadhyay, Pilgrim, Vidal. Information Maximization Perspective of Orthogonal Matching Pursuit with Applications to Explainable AI. NeurIPS 2023.

CLIP-IP-OMP: Details



[1] Chattopadhyay, Pilgrim, Vidal. Information Maximization Perspective of Orthogonal Matching Pursuit with Applications to Explainable AI. NeurIPS 2023.

Summary of the Information Pursuit Framework

- **Q1: How do we define the set of queries?**
  - Defined by domain experts [1].
  - Defined by large language models [4].
- **Q2: Given an input and a query, how do we answer the query?**
  - Train classifiers on data annotated with query answers by task experts [1].
  - Use domain-specific pre-trained large vision language models [4].
- **Q3: How do we select queries that form the explanation?**
  - **Information Pursuit**: Select smallest number of queries that are sufficient for prediction using Generative IP [1], Variational IP [2], and OMP [3].

[1] Chattopadhyay, Slocum, Haeffele, Vidal, Geman. Interpretable by design: Learning predictors by composing interpretable queries. TPAMI 2022.
[2] Chattopadhyay, Chan, Haeffele, Geman, Vidal. Variational Information Pursuit for Interpretable Predictions, ICLR 2023.
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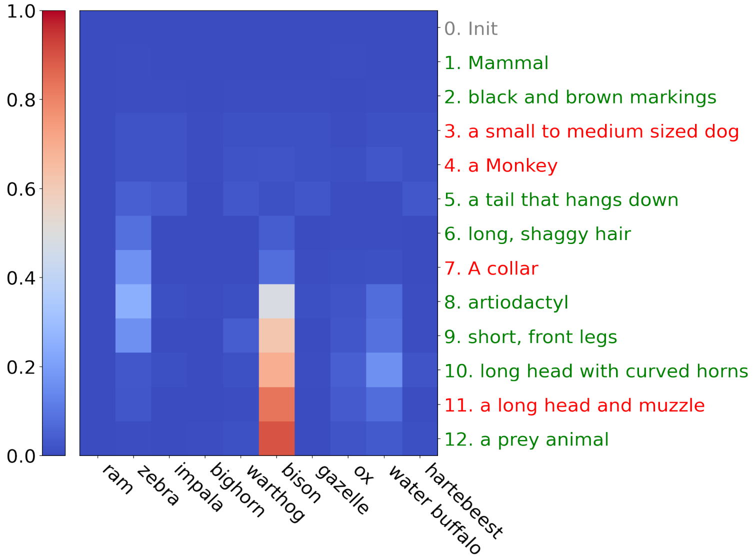
[5] Chattopadhyay, Haeffele, Vidal, Geman. Performance Bounds for Active Binary Testing with Information Maximization. ICML 2024.

Applications

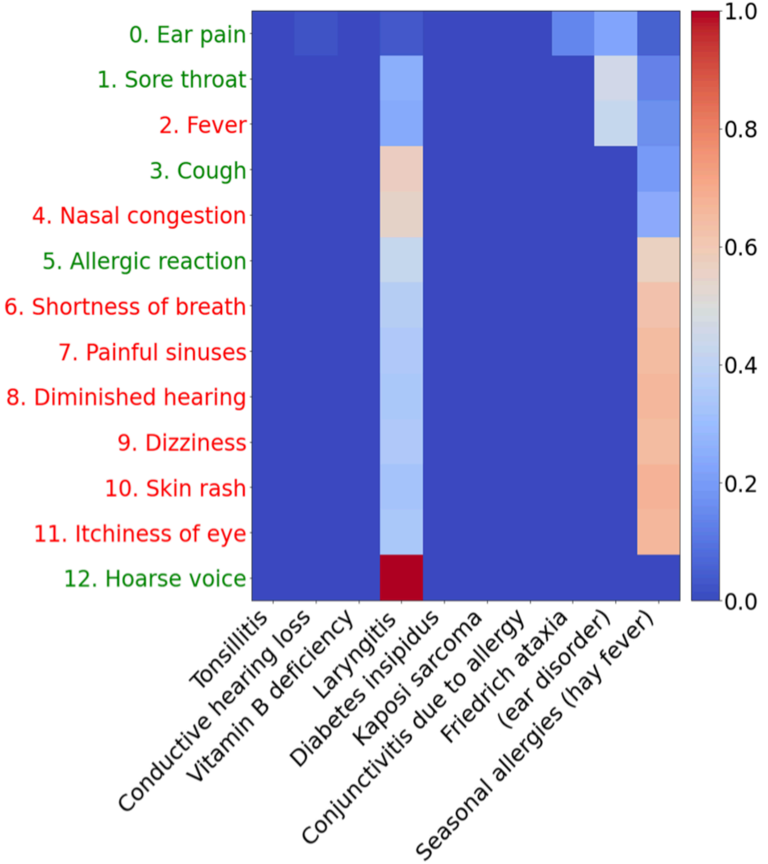
Interpretable Image Classification by V-IP

- **Task**: Image classification.
- **Query set**: Queries about presence or absence of different semantic concepts.
- **Dataset**: ImageNet
  - 1000 classes

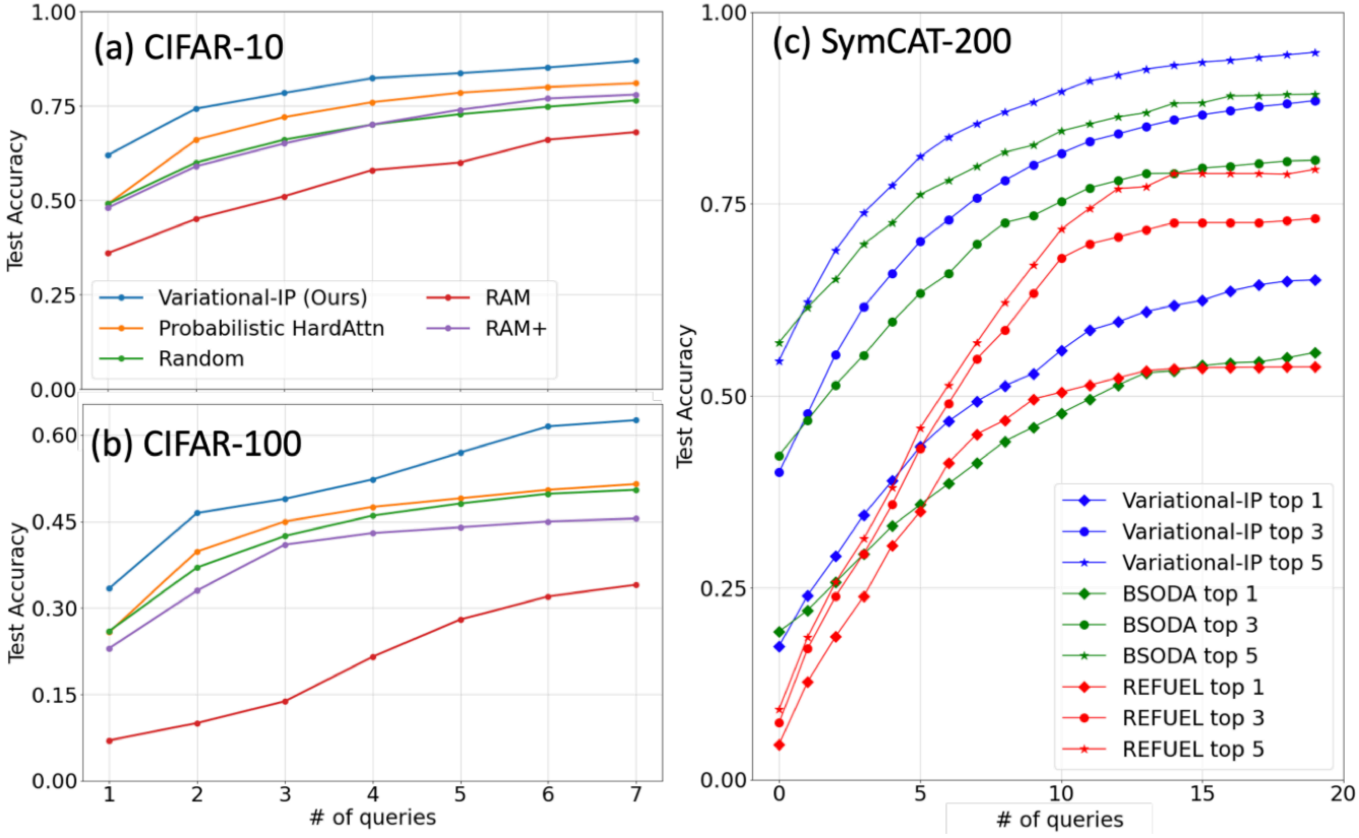


Interpretable Medical Diagnosis by VI-P

- **Task**: Disease diagnosis.
- **Query set**: Queries about presence or absence of different symptoms.
- **Dataset**: SymCAT-200
  - 1.1M doctor-patient dialogues about 326 symptoms indicative of 200 diseases.
  - Each dialogue: 2-3 symptoms per patient.
  - 326 binary queries, one per symptom.



Accuracy Versus Number of Queries



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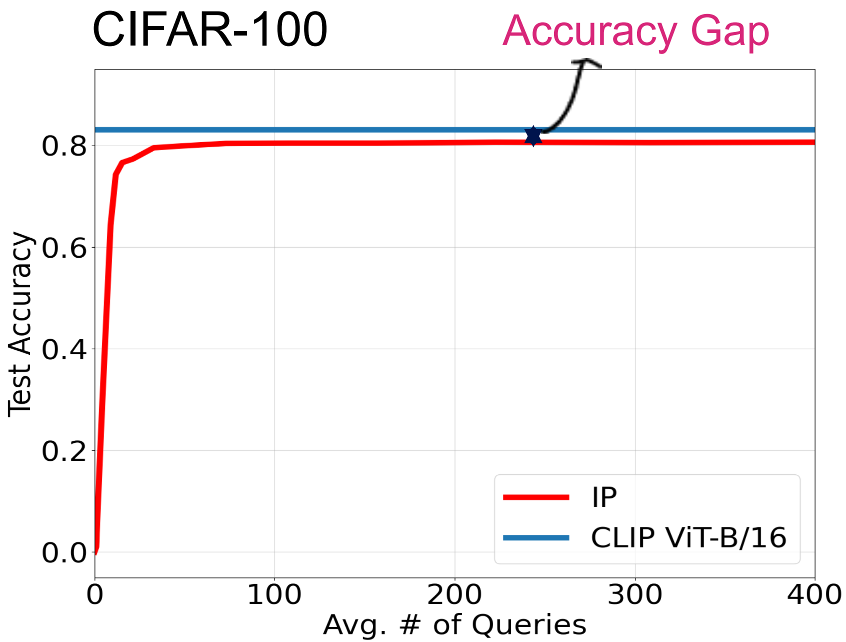
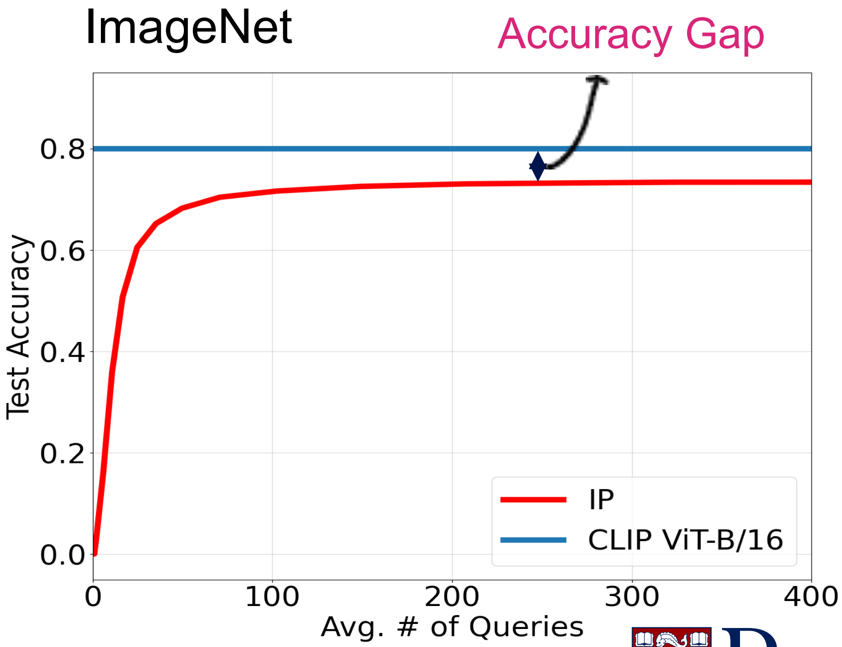
Accuracy-Explainability Tradeoff

- How far is interpretable-by-design from black-box model performance





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Interpretable Radiological Report Classification

- **Task**: Predict disease label in a radiological report.
- **Query set**: Queries about presence or absence of facts in a radiology report.
- **Dataset**: MIMIC-CXR
  - Data: 227,827 reports.
  - Queries are binary questions, one for each possible fact.
  - The task is to predict the disease label.

Interpretable Radiological Report Classification

- **Q1: How do we define the set of queries?**
  - Leverage LLMs and medical knowledge to extract 591,920 facts from 227,827 reports in the MIMIC-CXR dataset [1].
- **Q2: How do we answer a query for a given input?**
  - Leverage LLMs and medical knowledge to verify if a fact is present in a radiology report [2].
- **Q3: How do we select the best queries to form an explanation?**
  - Select smallest number of facts that are sufficient for disease prediction [2] using Variational IP [3,4].

[1] Messina, Vidal, Parra, Soto, Araujo. Extracting and Encoding: Leveraging LLMs and Medical Knowledge to Enhance Radiological Text Representation. ACL 2024.
[2] Ge, Chan, Messina, Vidal. Information Pursuit for Interpretable Classification of Chest Radiology Reports. ArXiv 2025.
[3] Chattopadhyay, Chan, Haeffele, Geman, Vidal. Variational Information Pursuit for Interpretable Predictions. ICLR 2023.
[4] Chattopadhyay, Chan, Vidal. Bootstrapping Variational Information Pursuit with Foundation Models for Interpretable Image Classification. ICLR 2024.

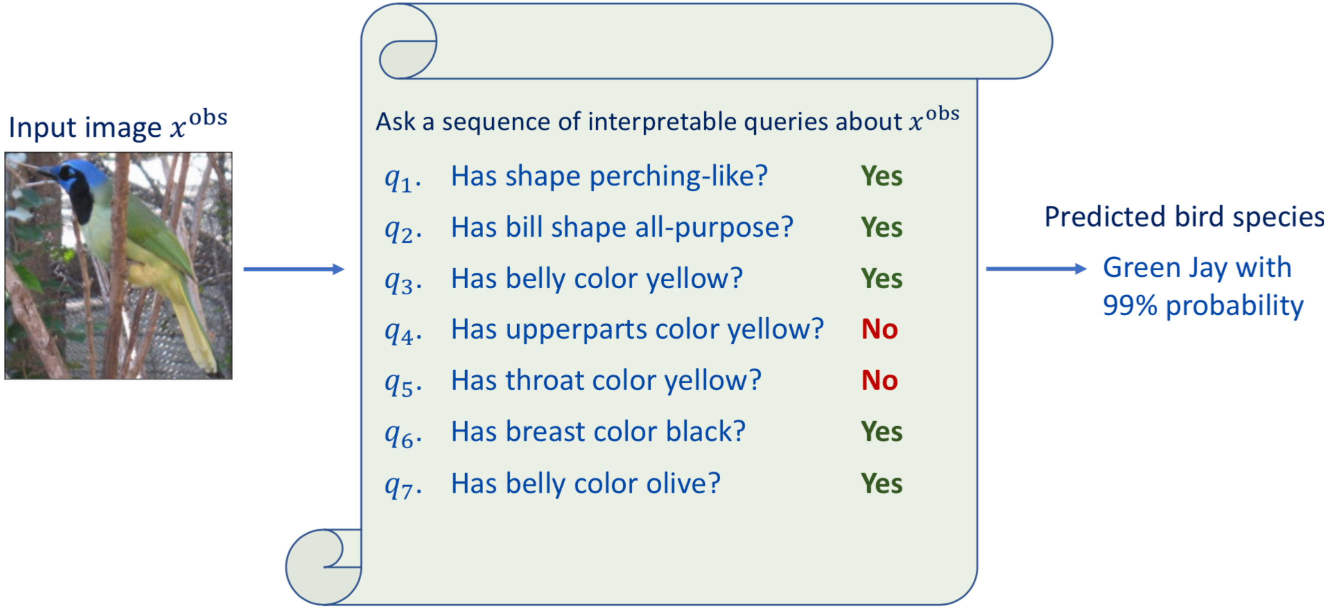
Interpretable Radiological Report Classification

- Average precision (AP) and F1 score of IP-CRR on six binary prediction tasks:
  - Lung Opacity (LO), Calcification of the Aorta (CA), Support Devices(SD),
  - Cardiomegaly(CM), Pleural Effusion(PE), and Pneumonia(PN).

Methods	AP						F1					
	LO	**CA**	**SD**	**CM**	**PE**	**PN**	**LO**	**CA**	**SD**	**CM**	**PE**	**PN**
CXR-BERT (FT-Last)	0.900	0.361	0.969	0.864	0.945	0.449	0.829	0.223	0.912	0.789	0.887	0.449
CXR-BERT (FT-All)	0.984	0.992	0.970	0.964	0.962	0.641	0.987	0.991	0.978	0.982	0.953	0.541
Flan-T5-large	0.527	0.073	0.445	0.380	0.616	0.190	0.663	0.139	0.321	0.543	0.754	0.299
CBM	0.947	0.345	0.934	0.791	0.874	0.432	0.884	0.241	0.853	0.738	0.801	0.431
IP-CRR	0.972	0.578	0.959	0.892	0.925	0.468	0.918	0.350	0.889	0.811	0.860	0.451

Summary

- Information Pursuit: an interpretable-by-design prediction framework.
- Generative model: use LLMs to define queries, VLMs to answer queries, and G-IP, V-IP, OMP to select queries and make predictions.



Open Questions

- **How to define interpretability?**
  - Hypothesis tests on the importance of a feature?
  - Minimum set of interpretable features that are sufficient for prediction?
  - What about causality-based explanations?

- **How to evaluate if a model is interpretable?**
  - Human evaluations?
  - Can humans predict a class based on explanation?
  - Benchmarks

Thank you

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