Handling Out-of-distribution Data in the Open World: Principles and Practices for Reliable AI

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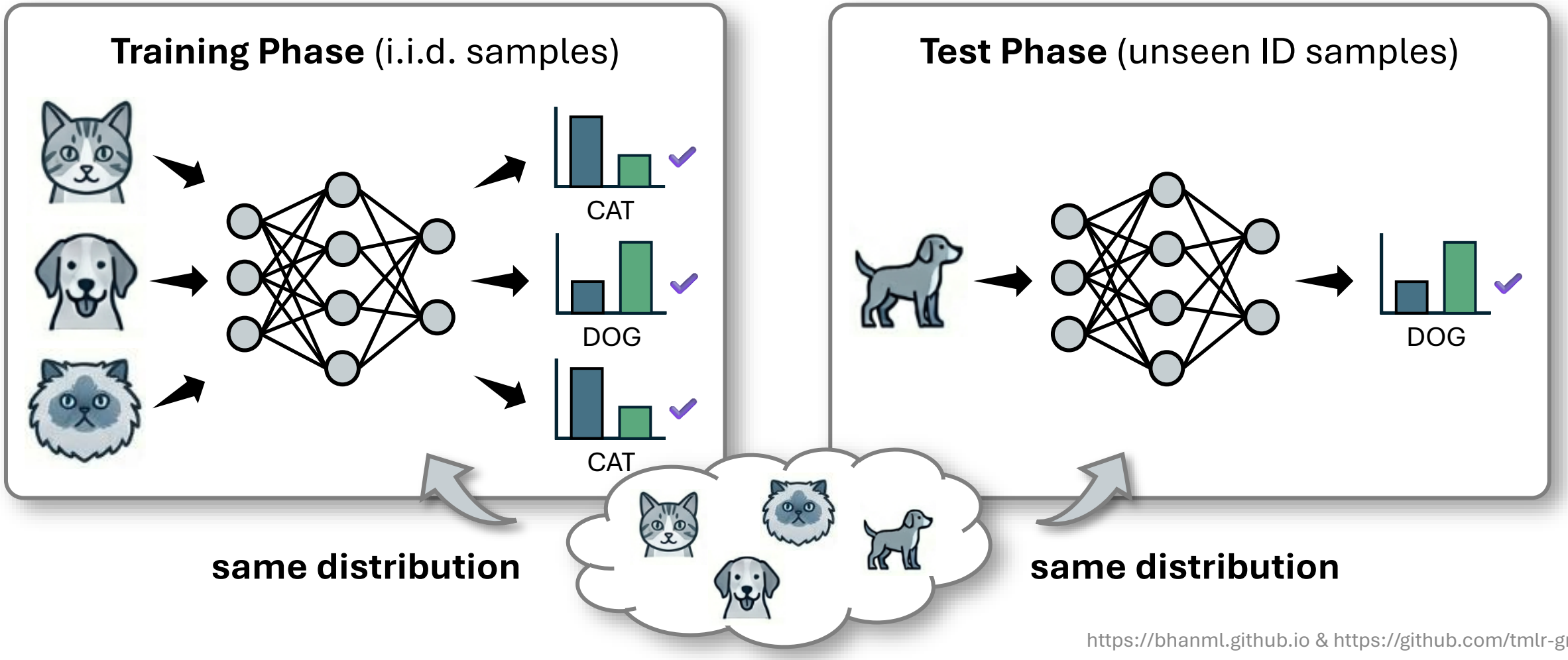
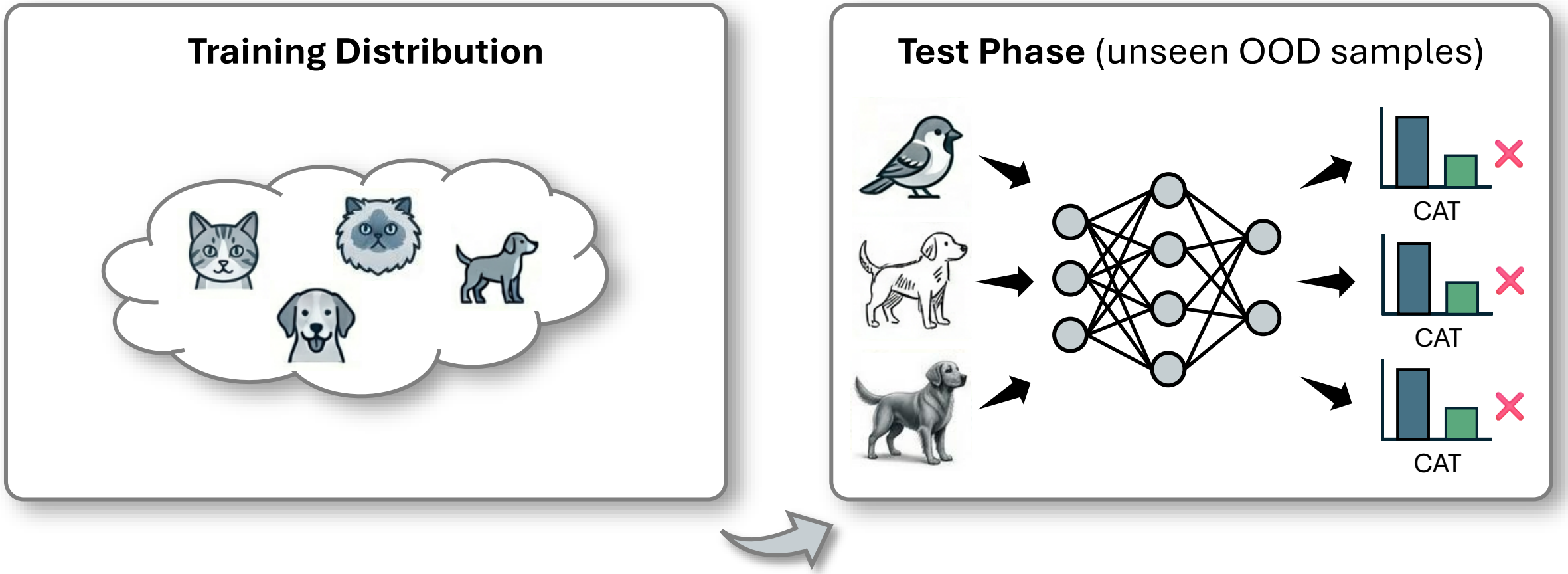
Model Generalization

Machine learning models are trained to generalize from a finite dataset to new, unseen i.i.d. samples drawn from the same distribution, i.e., **in-distribution (ID) data**.



Distribution Shifts

When test data distribution shifts, i.e., **out-of-distribution (OOD) data**, we can no longer guarantee the model performance (realistic dog and bird images are unseen).



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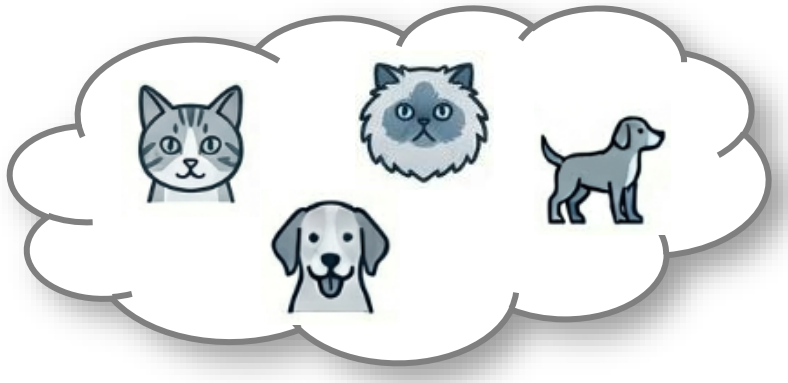
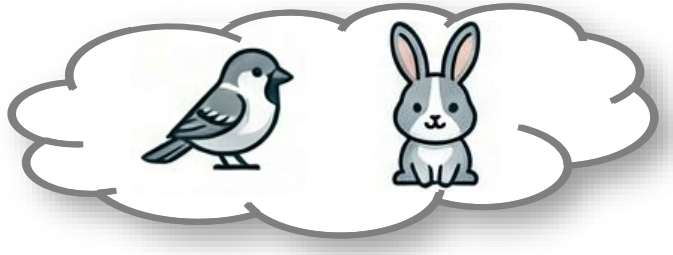
Training Distribution



Semantic Shift (different class, y shift)

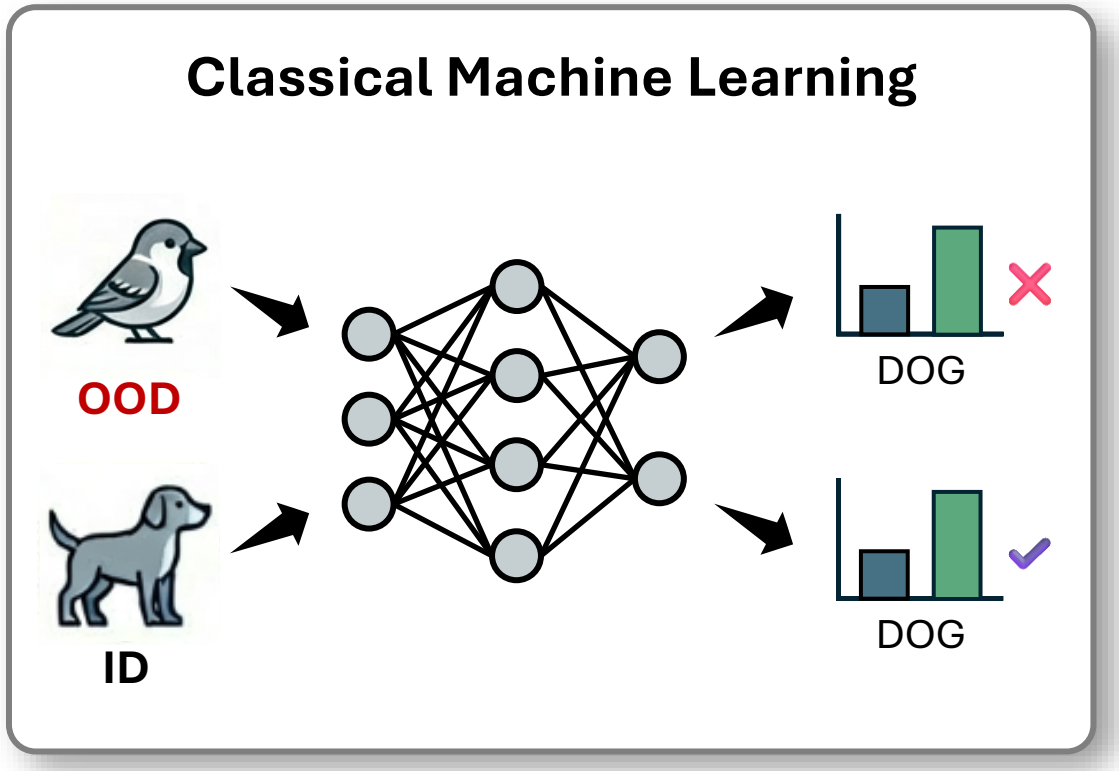


Covariate Shift (different style, x shift)

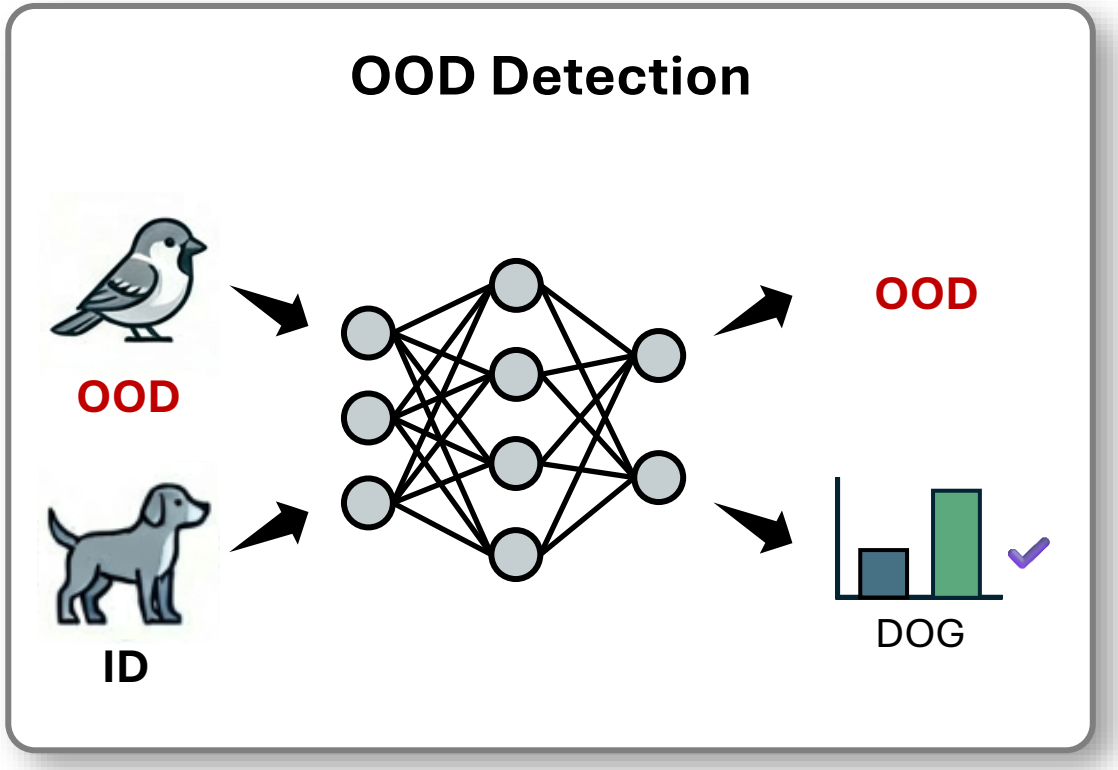
distribution shift

OOD Detection

Machine learning models should **detect semantic distribution shifts** and avoid making further label predictions (OOD generalization will consider covariate shifts).



No matter how strong the model is, **it will always make incorrect predictions**.



The model should **detect OOD data without further label predictions**.

OOD Detection in Autonomous Driving

Critical for road safety: Identifying **unknown scenarios or objects** to prevent accidents and ensure robustness.

Standard Vehicle (Known)

Horse-Drawn Carriage (OOD)

Fallen Tree on Road (OOD)

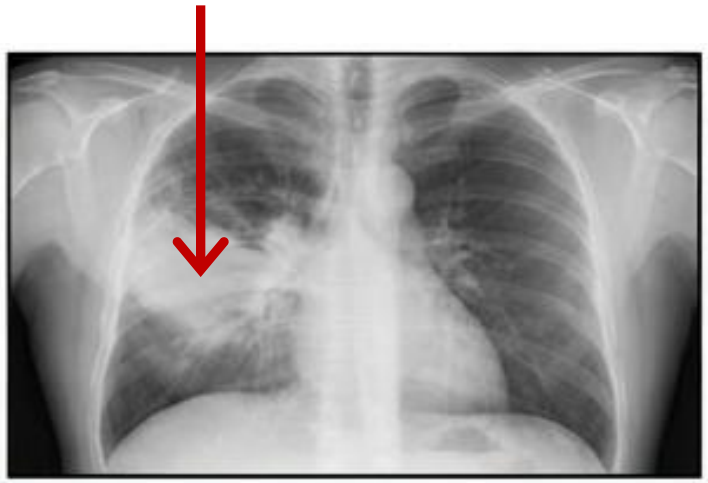
Models must recognize **novel objects** on the road to maintain safety boundaries.

The primary goal is to reliably flag OOD data, not to force **the vehicle prediction**.

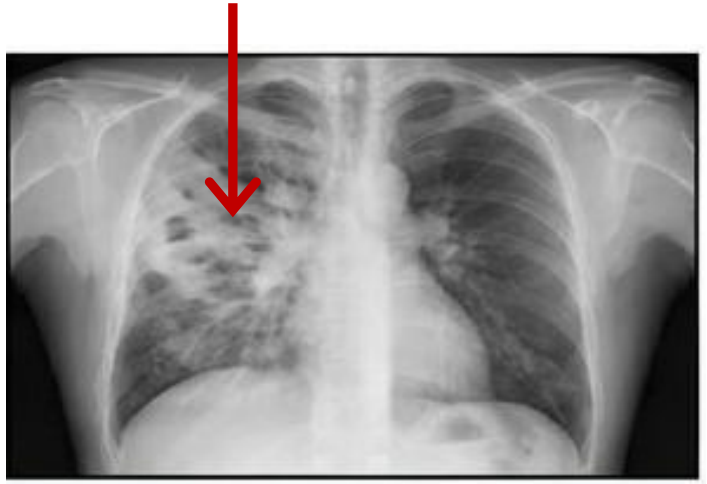
OOD Detection in Medical & Healthcare Systems

Critical for patient safety: Identifying **anomalies and unseen conditions** to prevent misdiagnosis and ensure reliability.

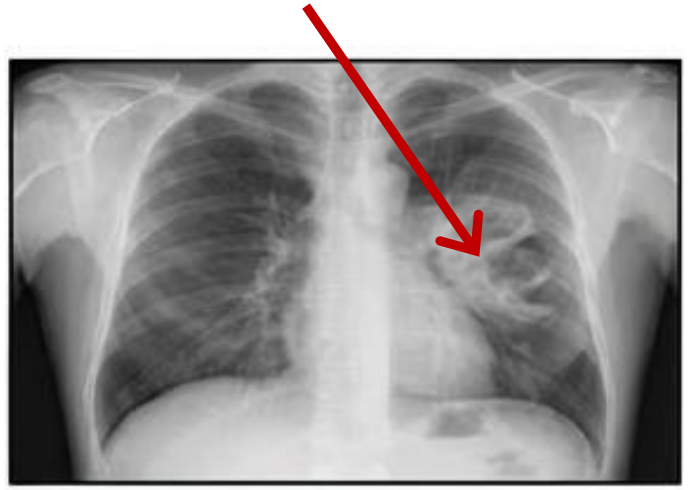
Common Pneumonia (Known)



Rare Tropical Disease (OOD)



Unseen Genetic Condition(OOD)



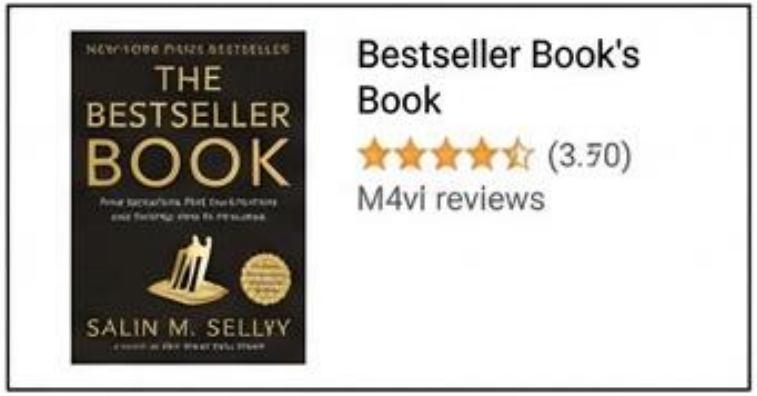
Models must recognize **unseen pathologies** to maintain the diagnostic integrity.

The primary goal is to reliably flag OOD cases for clinician review, not **automated diagnoses**.

OOD Detection in Recommender Systems

Critical for user trust: Identifying inputs **anomalous user-term interactions** to improve robustness and ensure fairness.

Popular Item (Known)



Niche Item (OOD)

Inappropriate Input (OOD)

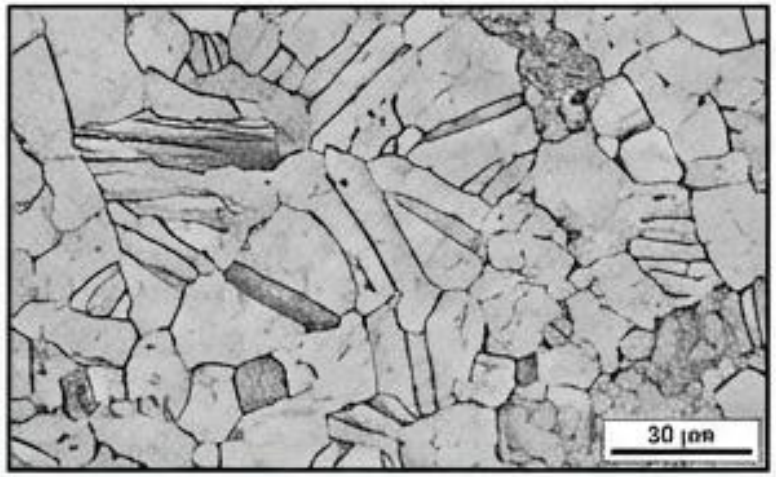
Models must recognize **novel user interests and item types** to maintain system integrity.

The primary goal is to reliably flag interactions for **review or adaptive recommendations.**

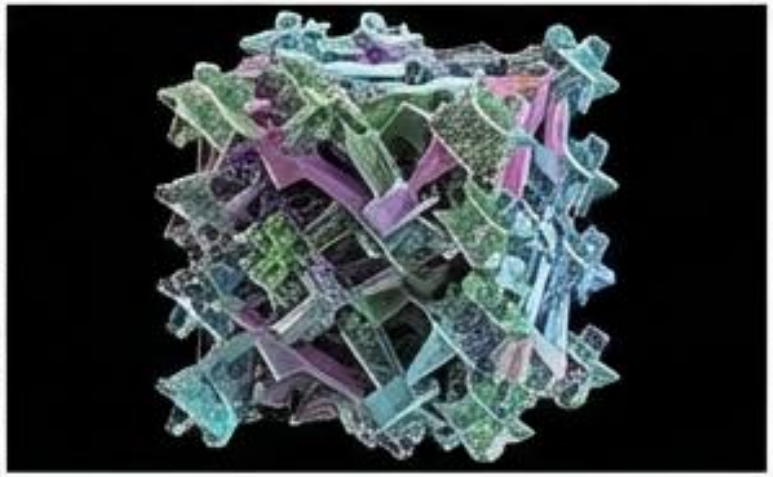
OOD Detection in Scientific Discovery

Critical for breakthroughs: Identifying anomalous data to **catalyse new theories and novel experiments**.

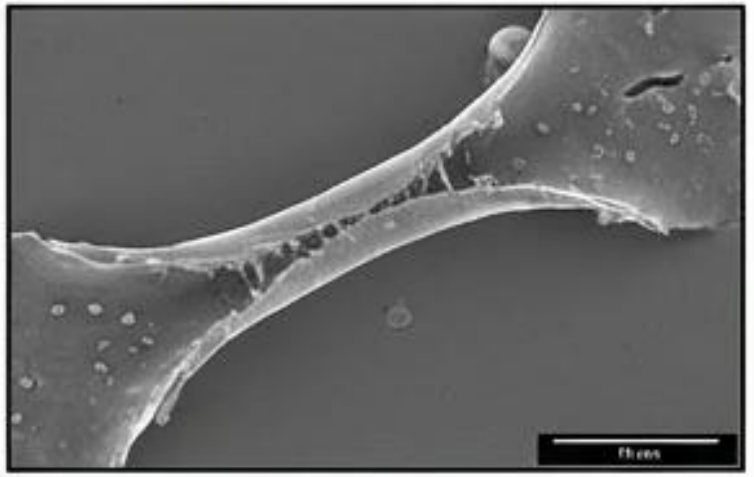
Common Alloy (Known)



Superconductor (OOD)



Bio-inspired Polymer (OOD)

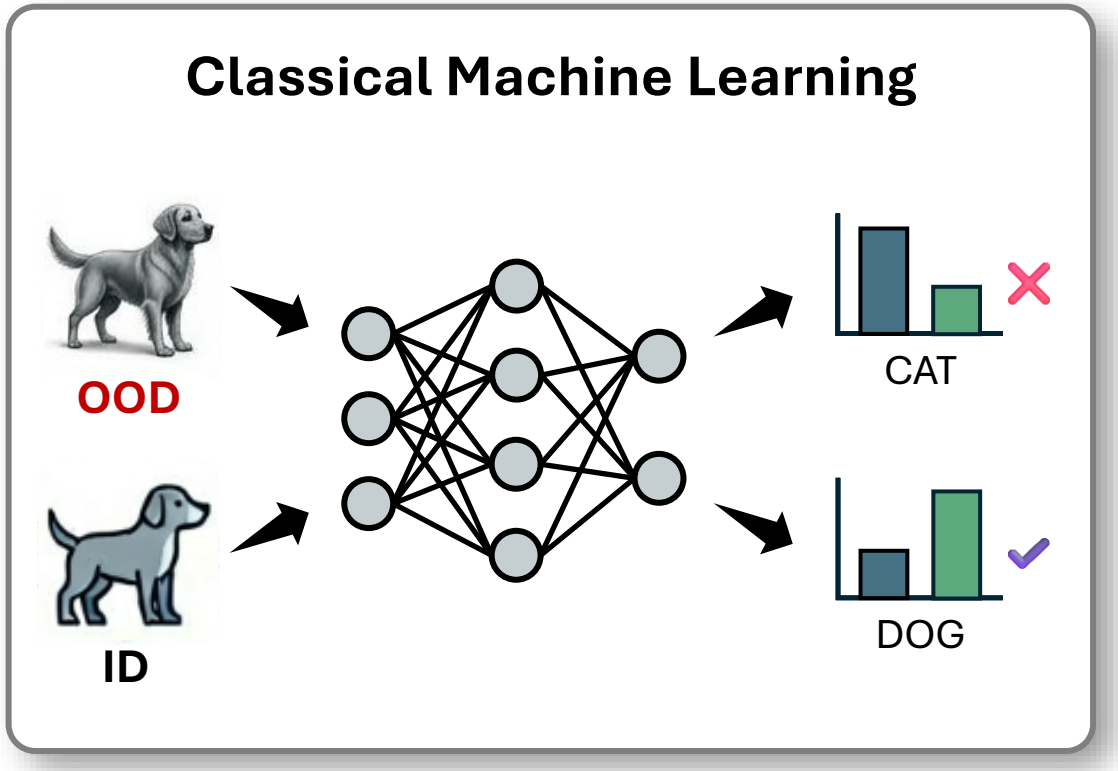


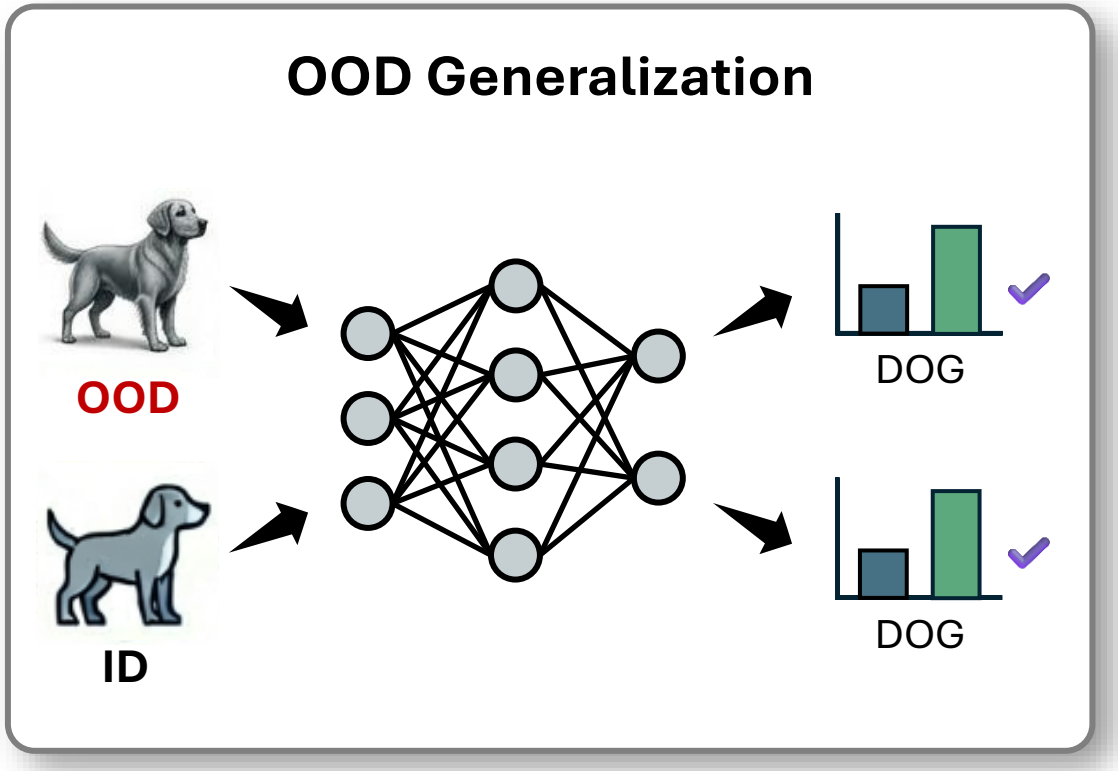
Models must flag **anomalous results and unexpected** patterns to guide research.

The primary goal is to highlight data for further investigation, not to force **fit existing categories**.

OOD Generalization

Machine learning models should **general well to data with covariate distribution shifts** and still produce correct label predictions.





If the model is strong enough, **it can make right predictions**.

The model should **generalize to unseen OOD data with right label predictions.**

OOD Generalization in Autonomous Driving

Beyond OOD detection that merely flags unseen objects, autopilot needs to generalize to **unseen scenarios** to prevent accidents and ensure safety under different conditions.

Standard Vehicle (Known)

Horse-Drawn Carriage (OOD)

Fallen Tree on Road (OOD)

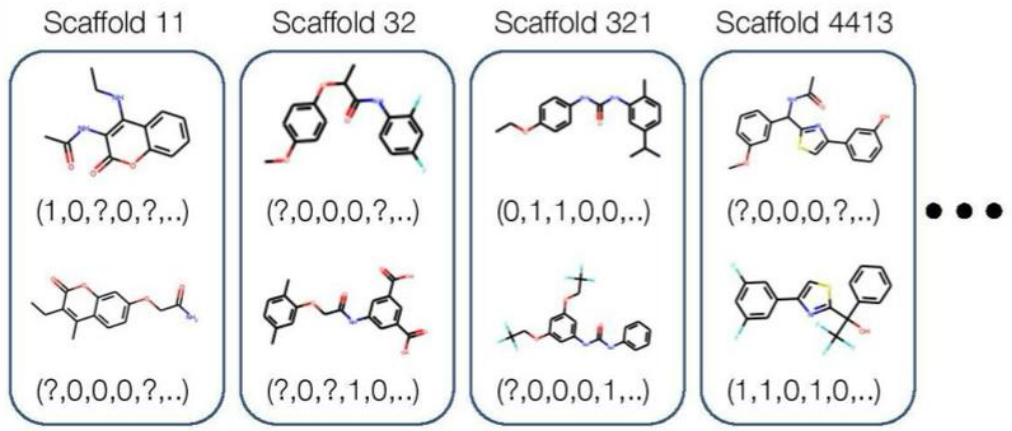
Training Environment

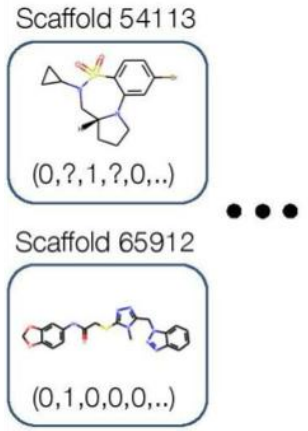
OOD Test Environments

Waymo Open Challenge

OOD Generalization in Drug Discovery

Critical for drug discovery: During the screening of candidate drugs, identifying **critical functional groups** that characterize the important biochemical properties of drugs, and avoid **spurious correlations of scaffolds** that take a large part of the molecule.





MolPCBA in wilds benchmark

ID molecules

OOD molecules with different scaffolds

OOD Generalization in Fairness

Critical for satellite imagery: In the analysis of images taken for different regions and subpopulations, immune to the spurious correlations associated with demographics.

Train			Test	
				
2002 / Americas	2009 / Africa	2012 / Europe	2016 / Americas	2017 / Africa
shopping mall	multi-unit residential	road bridge	recreational facility	educational institution

FMoW in wilds benchmark

Building/Land Type Classification

	Train			Test	
Satellite image (x)					
Country / Urban-rural (d)	Angola / urban	Angola / rural	Angola / urban	Kenya / urban	Kenya / rural
Asset index (y)	0.259	-1.106	2.347	0.827	0.130

PovertyMap in wilds benchmark

Poverty Estimation

https://bhanml.github.io & https://github.com/tmlr-group

OOD Generalization in Multimodal Alignment

Critical for hallucination mitigation of multimodal foundation models: Aligning concepts from multiple modalities and avoid multimodal spurious correlations.

Ice Bear in Snow (common) CLIP ACCU: 80.25

Ice Bear in Grass (counter) CLIP ACCU: 9.17

Tutorial Organization

30 mins — **Opening, Background, and Key Insights** (Prof. Bo Han)
Introducing the tutorial goals and real-world motivations.

1 hour — **Post-hoc OOD Detection** (Dr. Jianing Zhu)
*Perspectives on enhance OOD detection through better **logits**, **embedding**, and **distribution**.*

15 mins

1 hour — **OOD Detection Learning** (Dr. Qizhou Wang)
*Perspectives on enhance OOD detection through better **representation**, **calibration**, and **classification**.*

15 mins

1 hour — **OOD Generalization** (Dr. Yongqiang Chen)
*Perspectives on enhance OOD generalization through causality, from better **representation**, **optimization**, to **benchmarking**.*

30 mins — **Q&A**

About Me

Prof. Bo Han

- **Current Roles**

  Associate Professor in Machine Learning and **Director** of TMLR group at HKBU.

  BAIHO Visiting Scientist of Imperfect Information Learning Team at RIKEN AIP, hosted by Prof. Masashi Sugiyama.

- **Professional Service & Recognition**

  Senior Area Chair for NeurIPS and ICML, **Area Chair** for ICLR, UAI, and AISTATS.

  Associate Editor for IEEE TPAMI, MLJ, and JAIR, **Editorial Board** for JMLR and MLJ.

  ACM Distinguished Speaker and **IEEE Senior Member**.

About Members

- **Dr. Jianing Zhu**

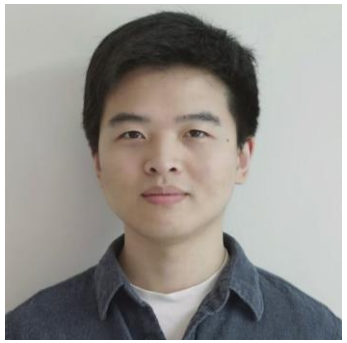
  Postdoctoral Fellow in the VITA group at UT Austin.

  Achieved PhD from the TMLR Group at HKBU.

- **Dr. Qizhou Wang**

  Postdoctoral Fellow in the Imperfect Information Learning Team at RIKEN AIP, working with Prof. Masashi Sugiyama.

  Achieved PhD from the TMLR Group at HKBU.



- **Dr. Yongqiang Chen**

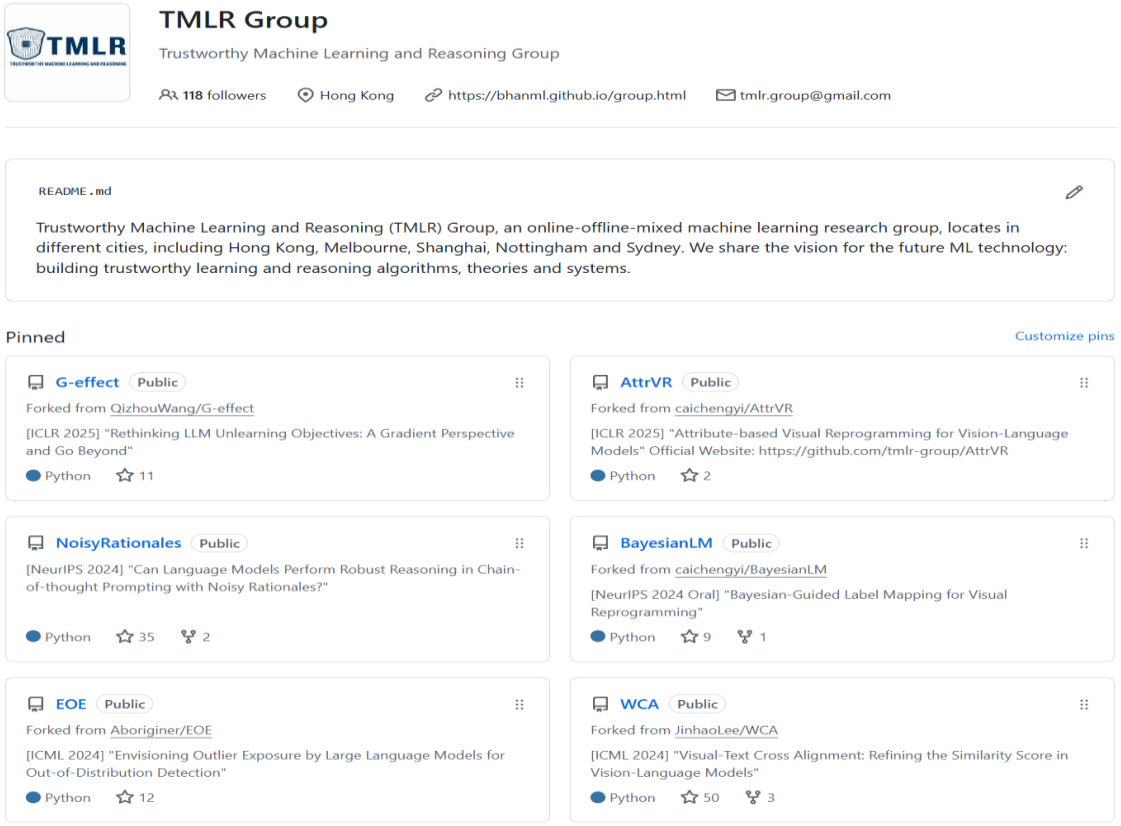
  Postdoctoral Fellow at CLeaR Group with Prof. Kun Zhang.

  Achieved PhD in CSE at CUHK in 2024, advised by Prof. James Cheng.

TMLR Group

TMLR Group, an online-offline-mixed **machine learning** research group, locates in different cities, including Hong Kong, Melbourne, Shanghai, Nottingham and Sydney.

We are welcoming the **synergetic collaboration** between yours and HKBU TMLR!!



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