On the Insights and Strategies for OOD Detection Learning

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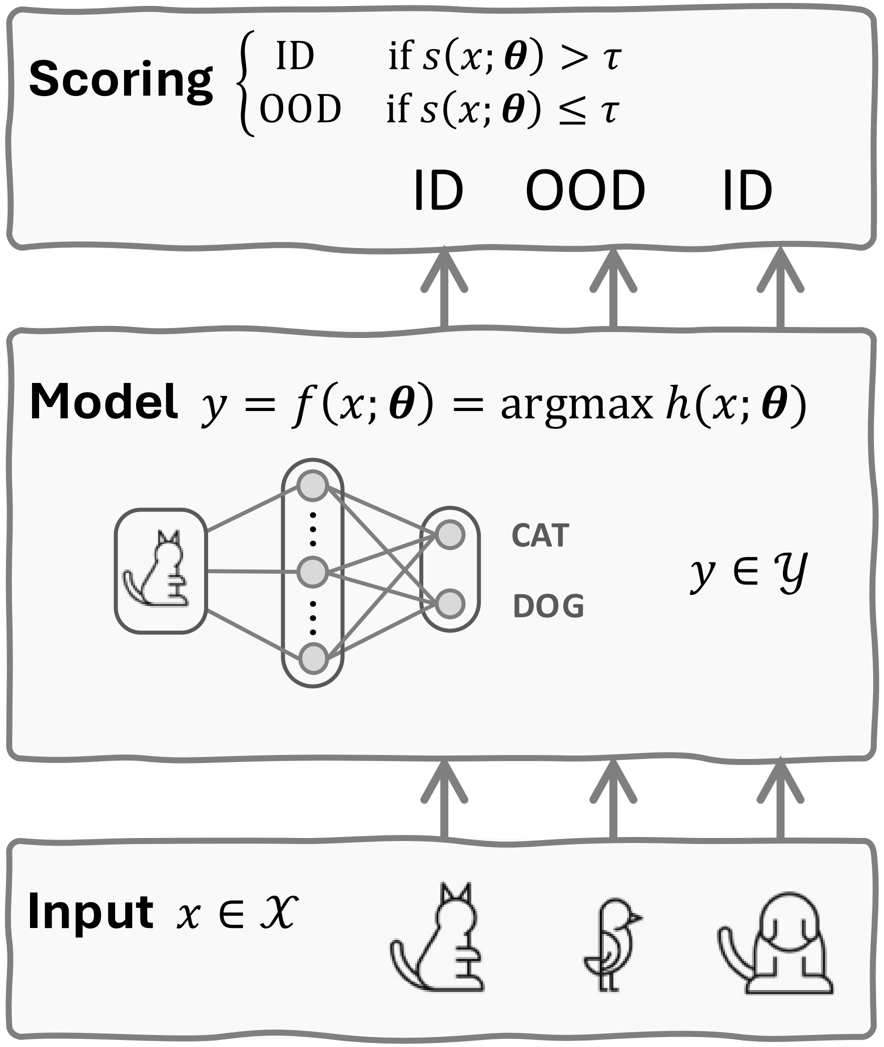
https://qizhouwang.github.io/homepage

Post-hoc OOD Detection: Review



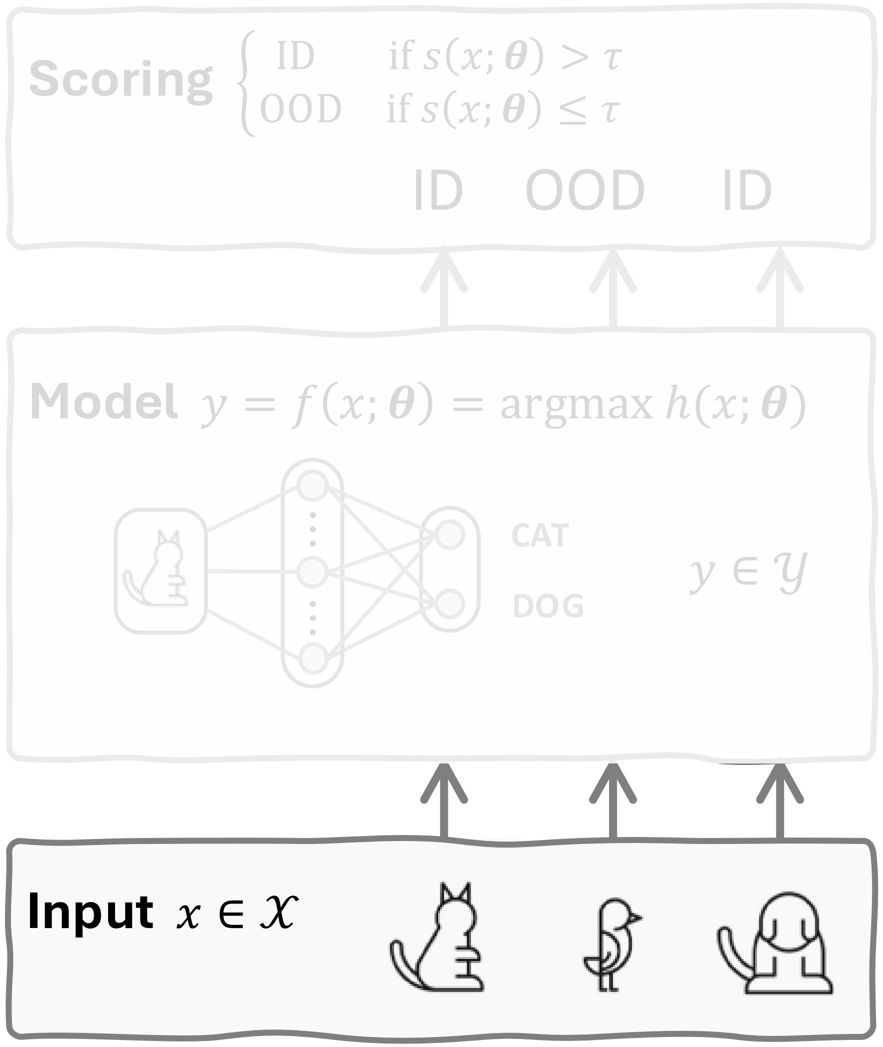
Semantic Shift: semantic relationship between inputs and labels changes.

ID OOD

Covariate Shift: feature distribution changes while labels stay within the label space.

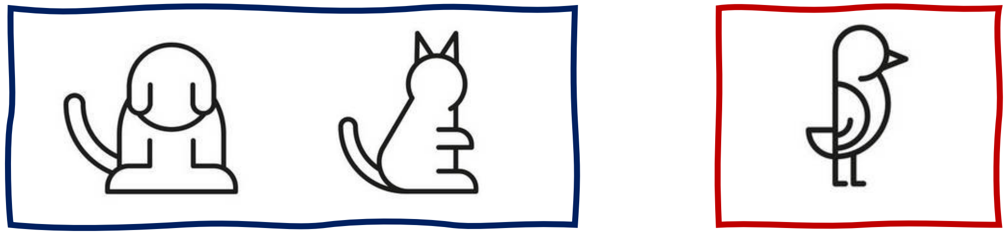
ID OOD

Post-hoc OOD Detection: Review



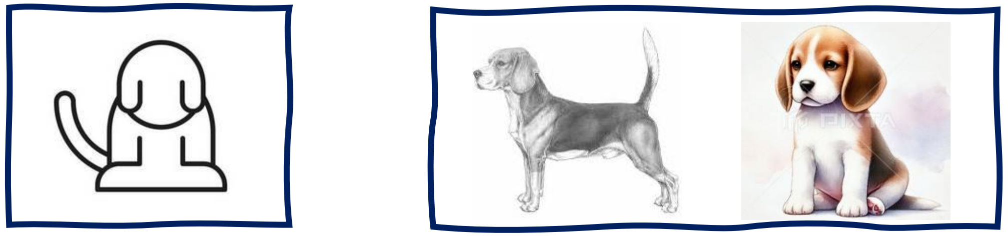
Interests of OOD detection

Semantic Shift: semantic relationship between inputs and labels changes.



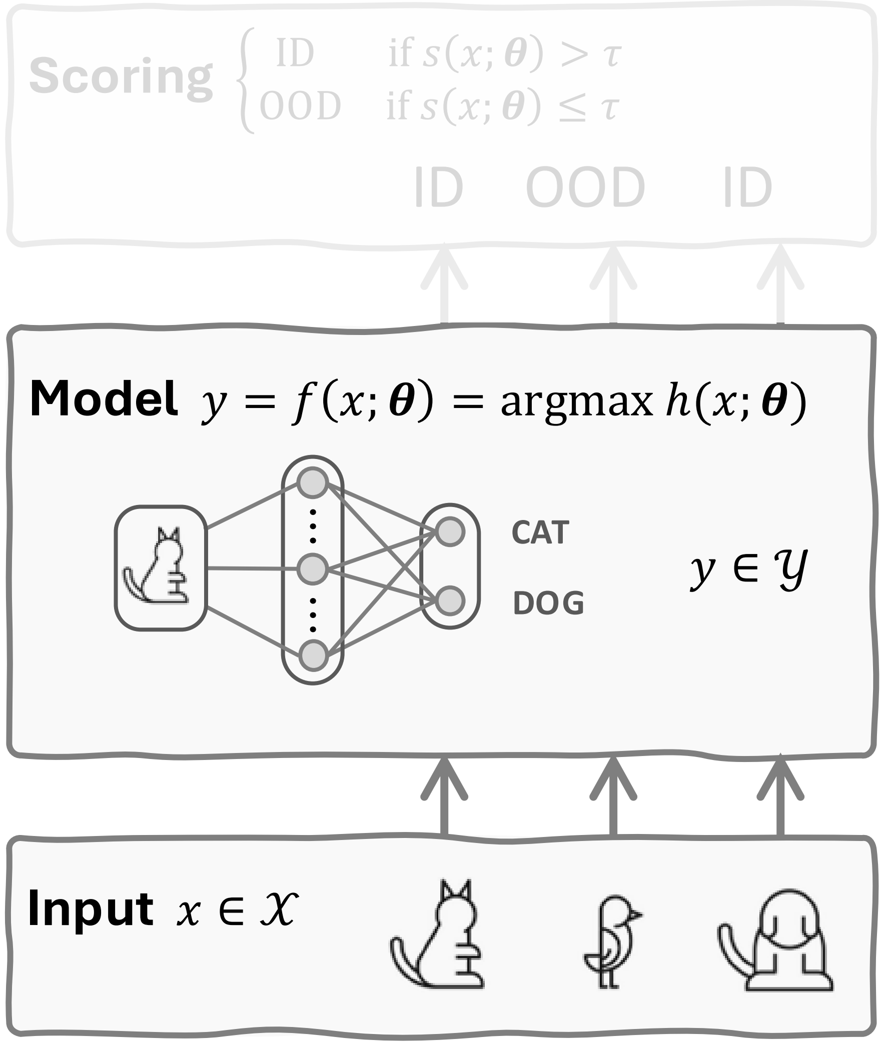
ID OOD

Covariate Shift: feature distribution changes while labels stay within the label space.

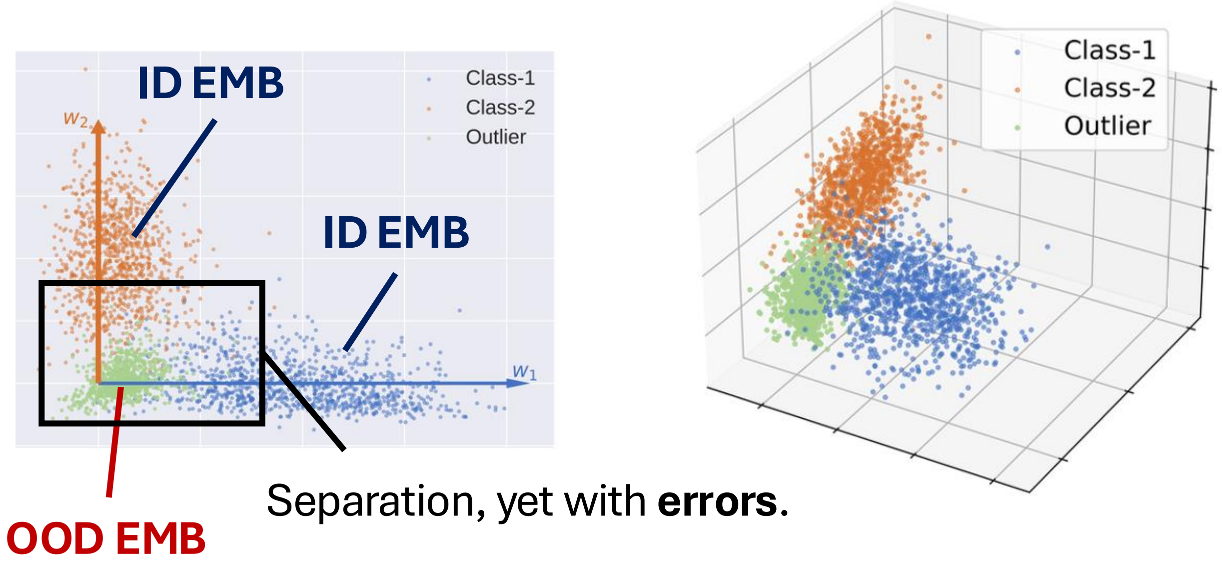


ID OOD

Post-hoc OOD Detection: Review



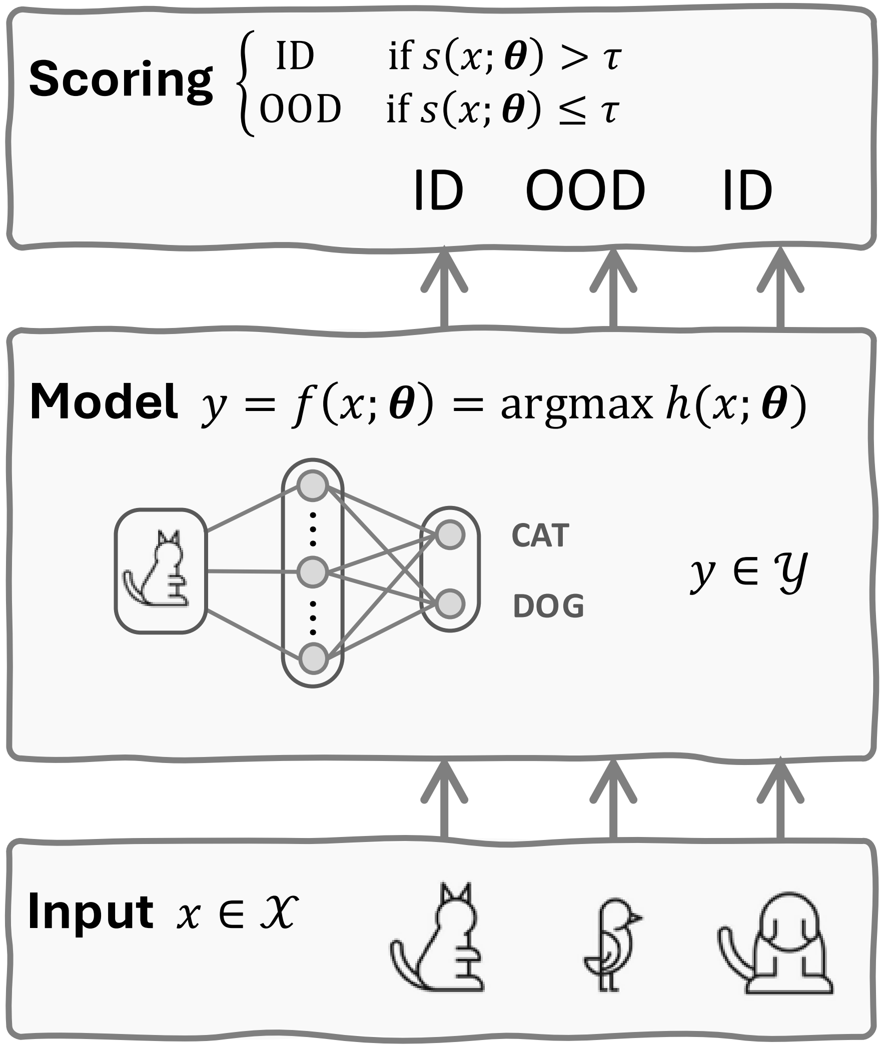
Pre-trained models can **separate ID and OOD data in embedding space** to some extent.



Figures of dimensional-reduced embeddings [a].

[a] Wu et al. Pursuing Feature Separation based on Neural Collapse for Out-of-Distribution Detection. In ICLR, 2025.

Post-hoc OOD Detection: Review



Model responses can be used to craft OOD scoring functions.

maximal softmax prediction

- **Output Level**, MSP [a]

$$s_{\text{MSP}}(x;\boldsymbol{\theta}) = \max_{\text{k}} \text{softmax}_{\text{k}}\, h(x;\boldsymbol{\theta})$$

k-th nearest neighbor

- **Embedding Level**, KNN [b]

$$s_{\text{KNN}}(x;\boldsymbol{\theta}) = \left\| h(x;\boldsymbol{\theta}) - z_{(k)} \right\|_2$$

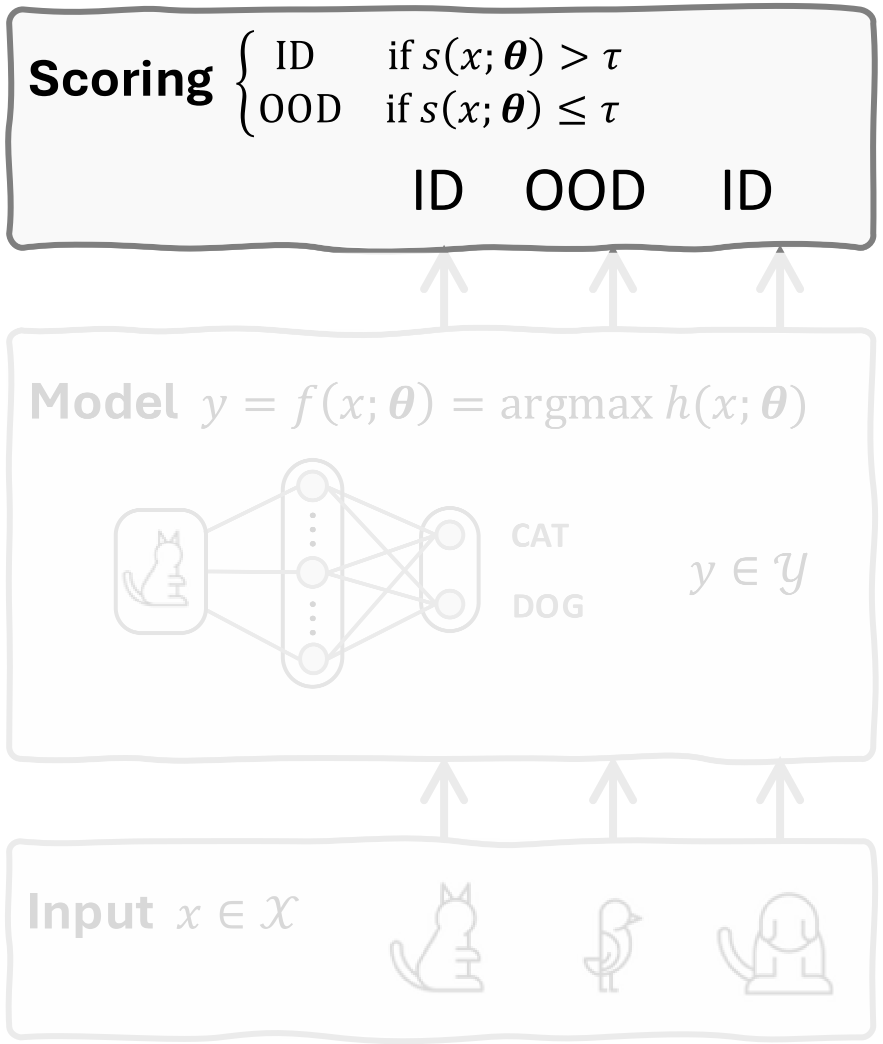
uniform distribution

- **Gradient Level**, GradNorm [c]

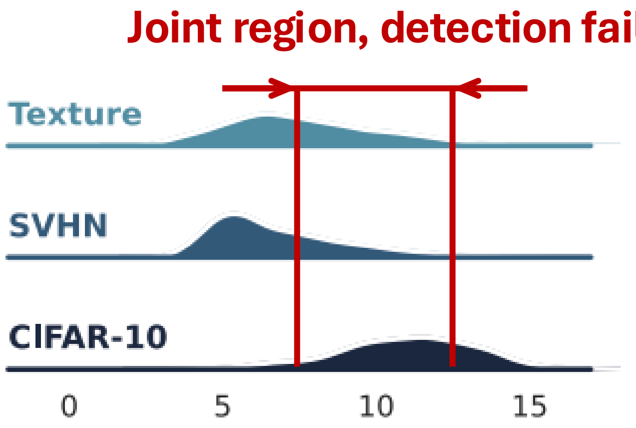
$$s_{\text{GN}}(x;\boldsymbol{\theta}) = \|\nabla_{\boldsymbol{\theta}} \text{KL}(u \| \text{softmax}(h(x;\boldsymbol{\theta})))\|_2$$

[a] Hendrycks et al. A Baseline for Detecting Misclassified and Out-of-Distribution Examples in Neural Networks. In ICLR, 2017.
[b] Sun et al. Out-of-Distribution Detection with Deep Nearest Neighbors. In ICML, 2022.
[c] Huang et al. On the Importance of Gradients for Detecting Distributional Shifts in the Wild. In NeurIPS, 2021.

Post-hoc OOD Detection: Challenges



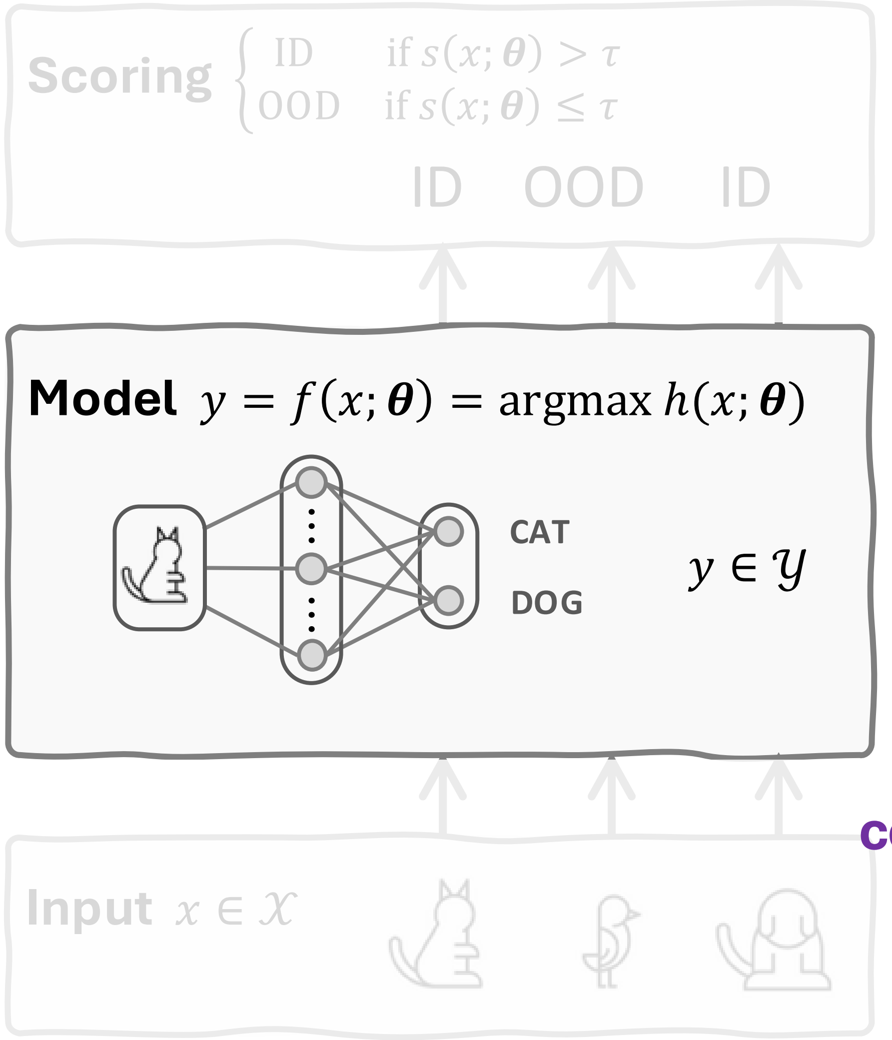
Post-hoc OOD detection often **makes mistakes**, failing to discern many ID and OOD patterns.



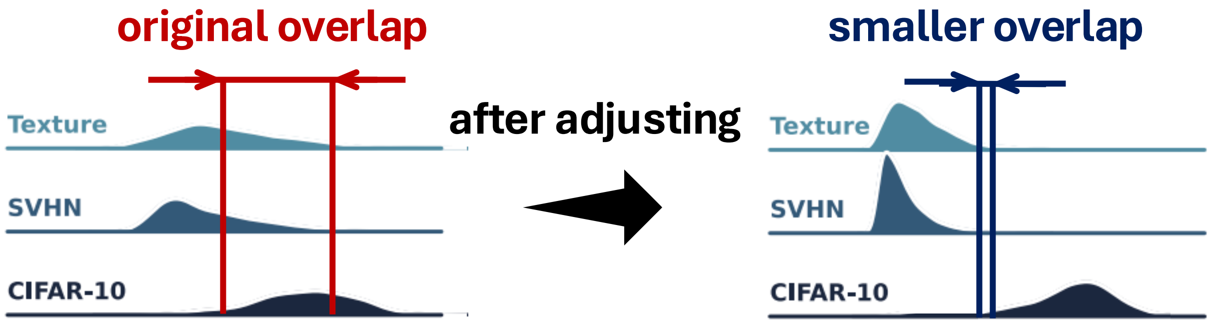
Figures of ID & OOD scoring distributions [a].

Explanations: For conventional-trained models, 1) their **representations** are not good enough, b) their **calibration** is inherently poor, and c) they cannot fully **classify** ID and OOD patterns.

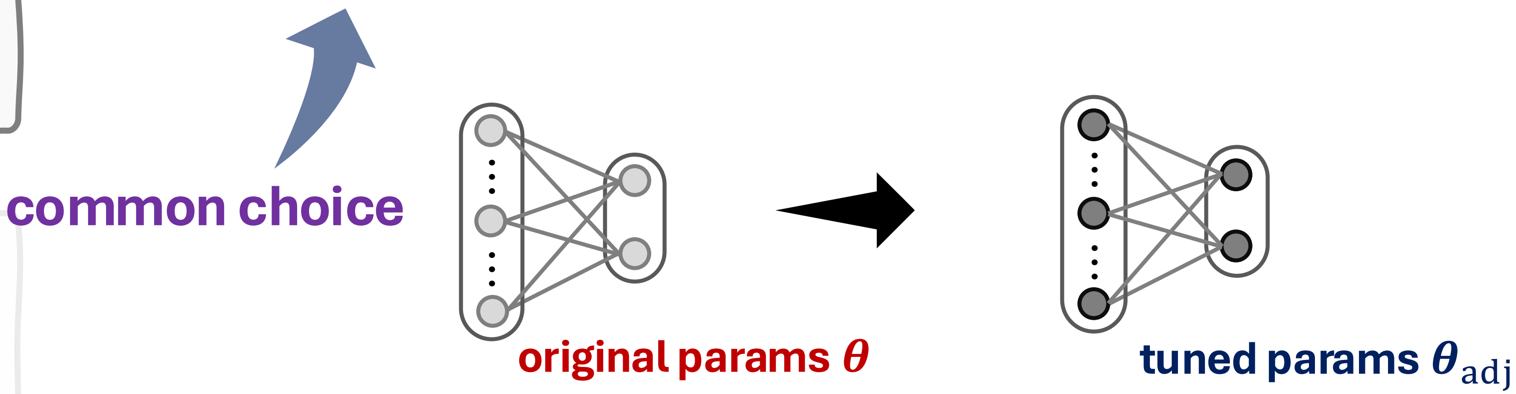
OOD Detection Learning: What to Adjust?



Adjust the system to improve OOD detection.



❖ **Model Level**, most works $s(x;\boldsymbol{\theta}) \rightarrow s(x;\boldsymbol{\theta}_{\text{adj}})$



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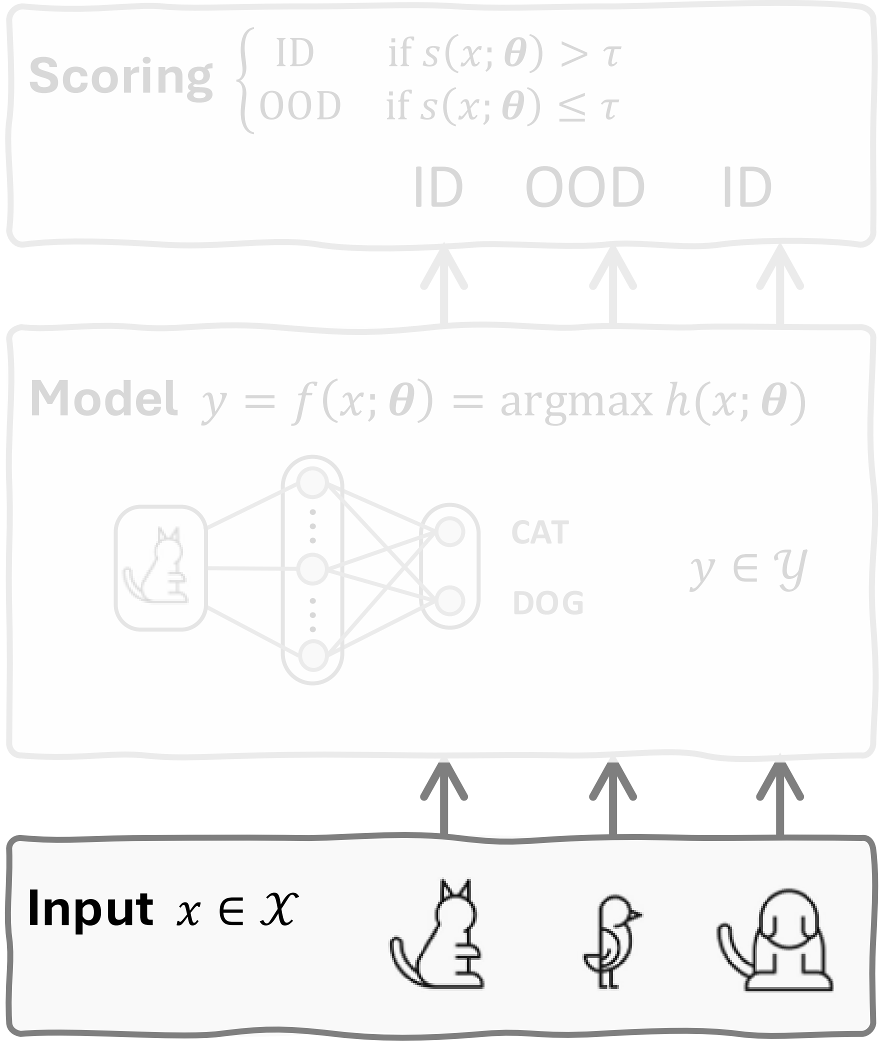

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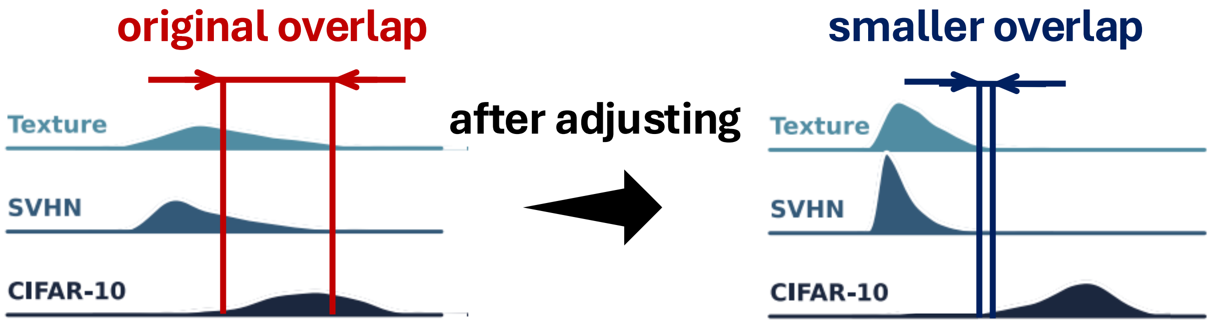
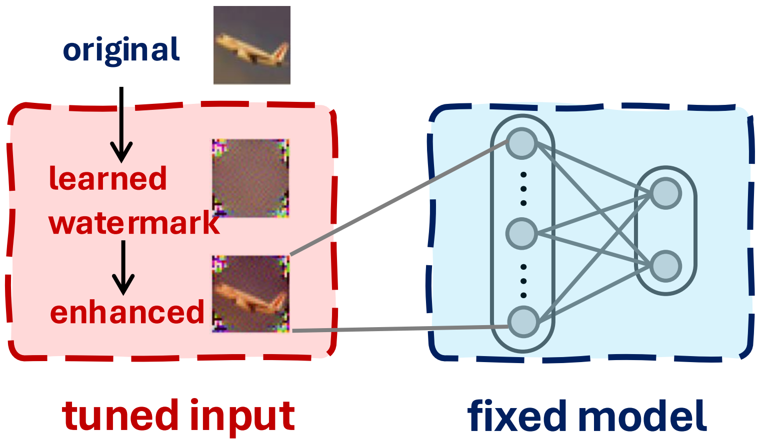


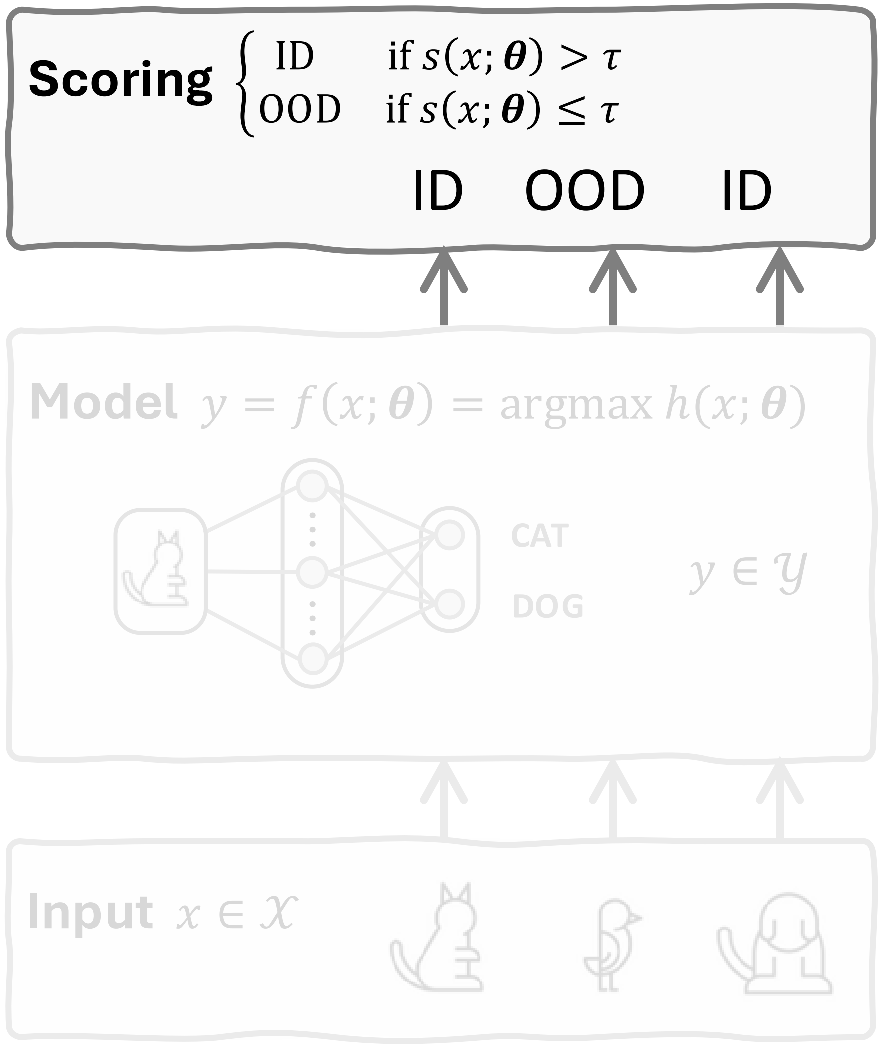
❖ **Input Level**, WM [a] $s(x;\boldsymbol{\theta}) \rightarrow s(x+w;\boldsymbol{\theta})$



- ❖ *Watermark is static, **tuned** to enhance OOD detection.*
- ❖ *The pre-trained model remains **fixed**.*

[a] Wang et al. Watermarking for Out-of-distribution Detection. In NeurIPS, 2022.

OOD Detection Learning: What to Adjust?



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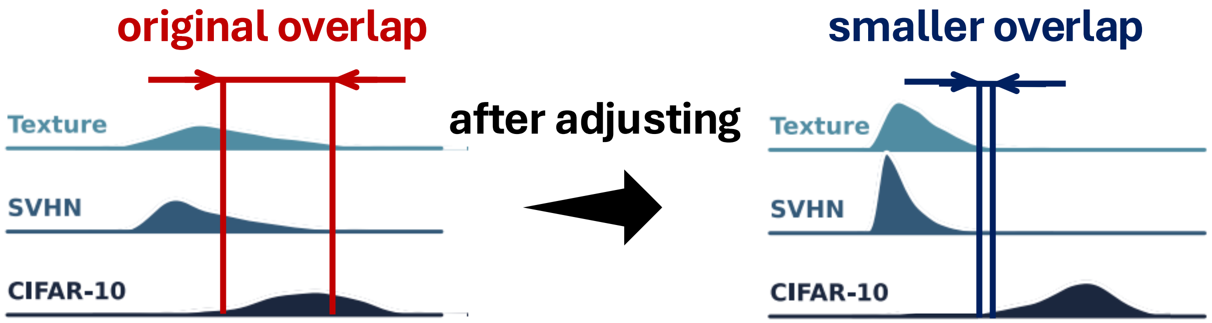
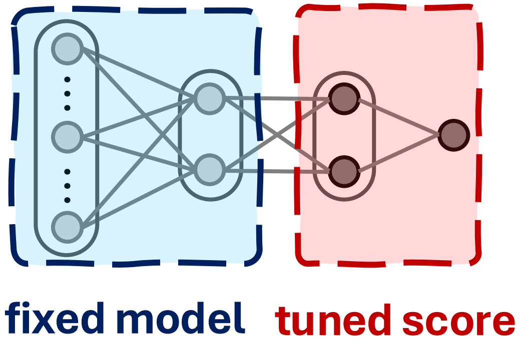


❖ **Score Level**, VOS [a] $s(x;\boldsymbol{\theta}) \rightarrow \boldsymbol{s}(h(x;\boldsymbol{\theta}), \boldsymbol{w})$



❖ *The scoring function introduces exact params to be **tuned**.*

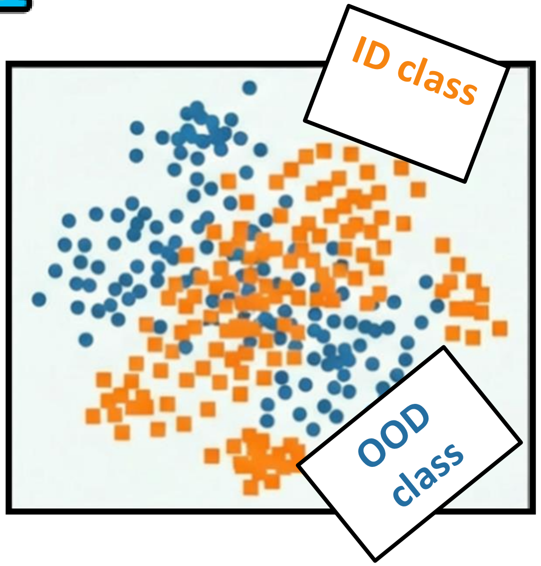
❖ *The pre-trained model remains **fixed**.*

[a] Du et al. Learning What You Don't Know by Virtual Outlier Synthesis. In ICLR, 2022.

OOD Detection Learning: How to Adjust?

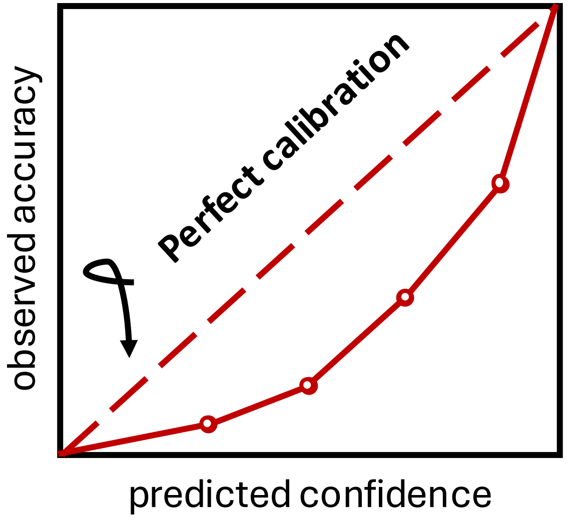
Let's recall **the drawbacks of post-hoc OOD detection:** For conventional-trained models, they have

Poor Representation



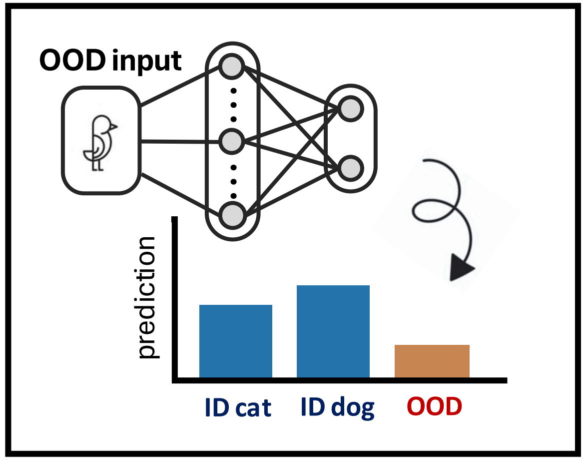
Data with **different semantics** may **not be perfectly separated** in the embedding space.

Poor Calibration



High model confidence does not correspond to **high model accuracy**.

Poor Classification



The model **predicts the wrong class**, despite the true class of being either ID or OOD.

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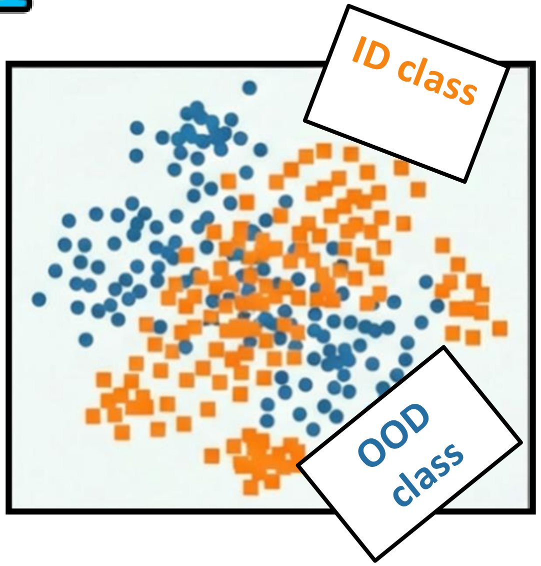

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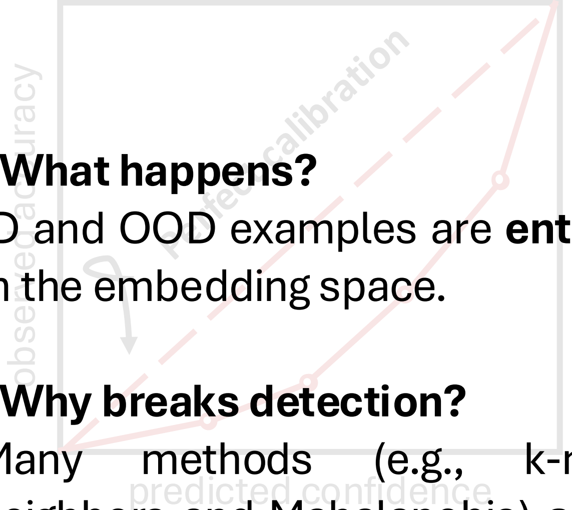

❖ **What happens?**
ID and OOD examples are **entangled** in the embedding space.

❖ **Why breaks detection?**
Many methods (e.g., k-nearest neighbors and Mahalanobis) **assume that OOD lies away from ID.**

not correspond to **high model accuracy**.

Poor Classification

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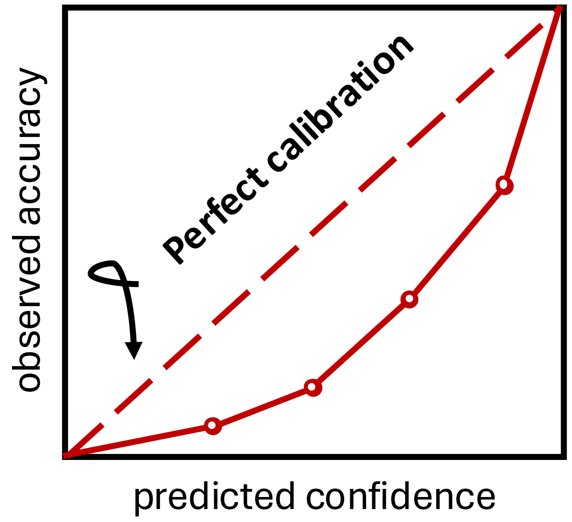

High model confidence does not correspond to **high model accuracy**.

Poor Classification

- **What happens?**
  Models produce **high confidence for wrong predictions**.
- **Why breaks detection?**
  Many methods (e.g., MSP) **use confidence-like scores.**

The model **predicts the wrong class**, despite the true class of being either ID or OOD.

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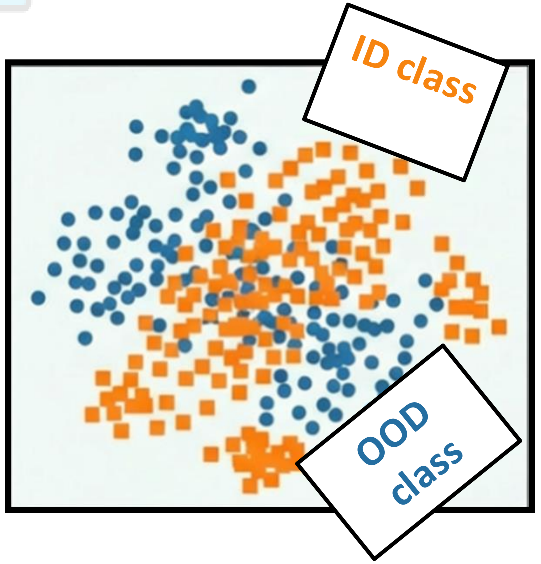

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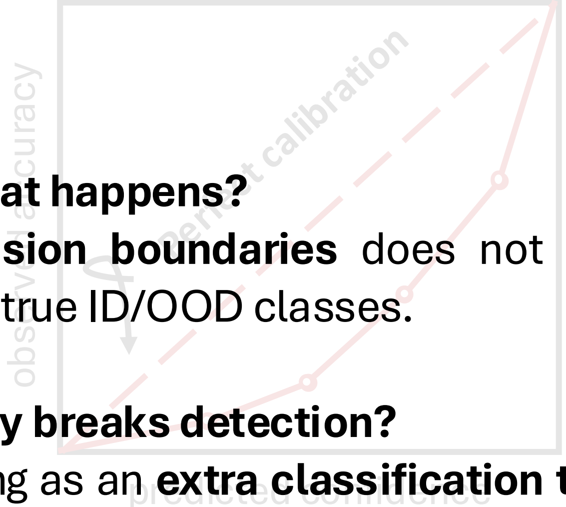
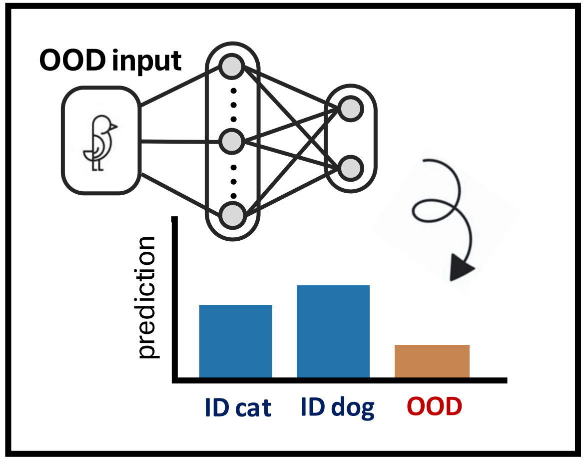


High model confidence does not correspond to **high model accuracy**.

❖ **What happens?**
Decision boundaries does not align with true ID/OOD classes.

❖ **Why breaks detection?**
Taking as an **extra classification task**, this classifier is not accurate.

Poor Classification



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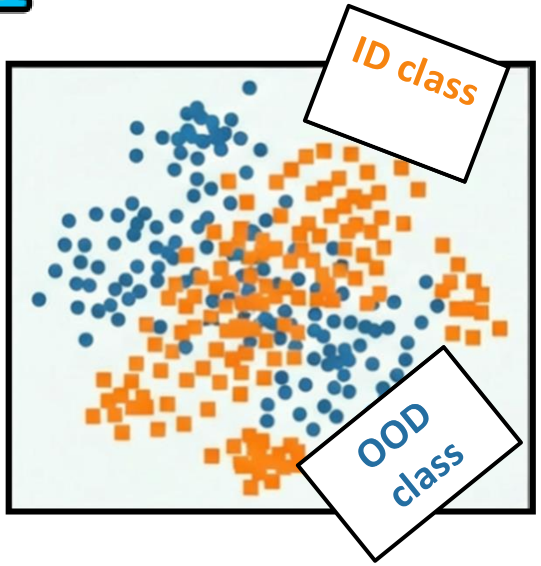

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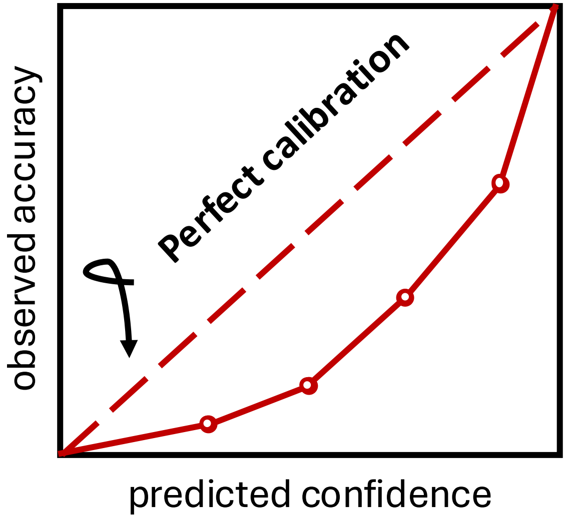

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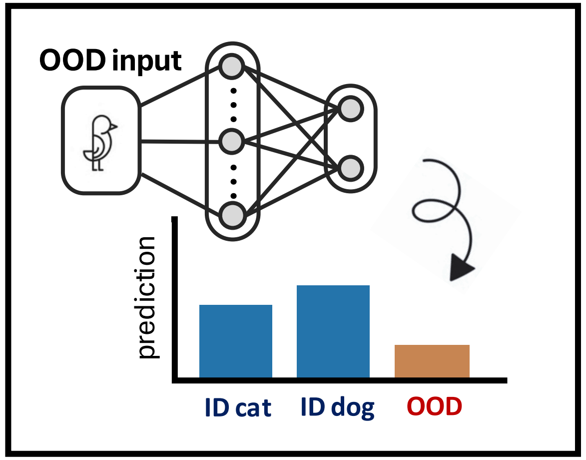

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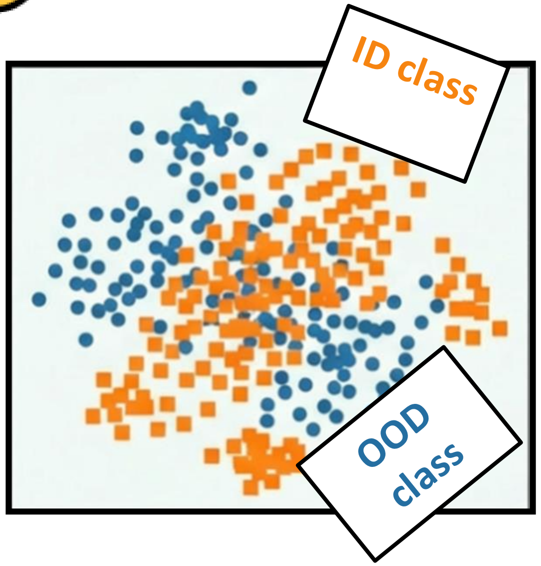
OOD Detection Learning: How to Adjust?

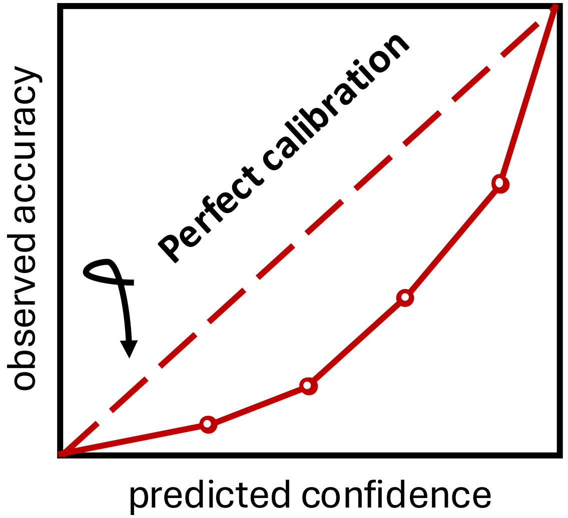
To **address the drawbacks** of post-hoc OOD detection, OOD detection learning can

Improve Representation



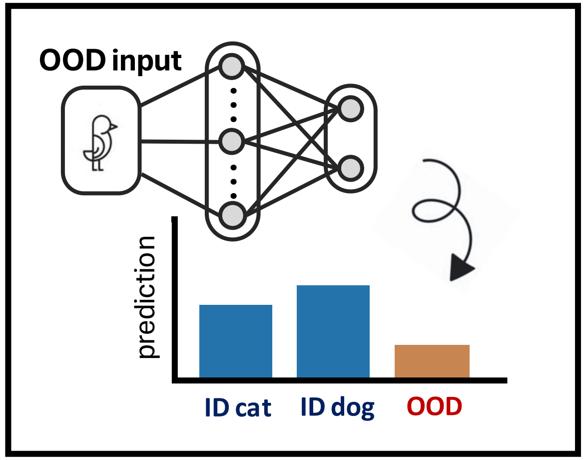
- **contrastive learning,**
- **reconstruction learning,**
- **pre-training,** et al.

Improve Calibration



- **Bayesian scoring,**
- **density regularization,**
- **calibration,** et al.

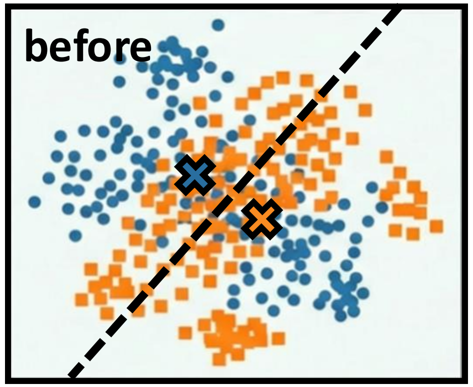
Improve Classification



- **outlier exposure,**
- **data augmentation,**
- **sample selection**, et al.

Representation: Overview

Conventional-trained Classifiers → **Representation-based OOD Learning**



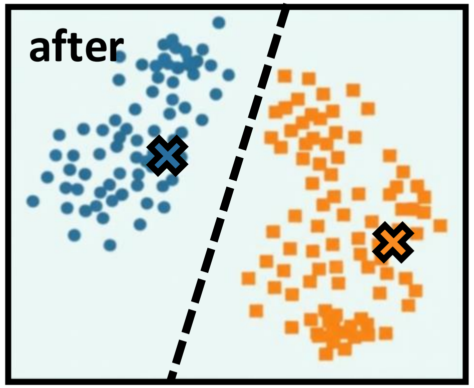
ID/OOD boundary

A simple OOD scoring : Nearest distances to K-means clustering.

$$s_{\mathrm{KM}}(x;\boldsymbol{\theta}) = \left\|h(x;\boldsymbol{\theta}) - \mu_{(x)}\right\|_2$$

nearest ID centroid

- ❖ make **no assumptions about the form of OOD data** will take or the type of downstream task.
- ❖ mainly learn patterns among training classes as a **shortcut to learn classification**.



Representations with different semantics are better separated.

- ❖ low intra-class variance
- ❖ high inter-class variance

Pretext tasks

- ❖ **Contrastive Learning**: CSI, SSD
- ❖ **Reconstruction Learning**: MOOD
- ❖ **Pre-training**: CLIP

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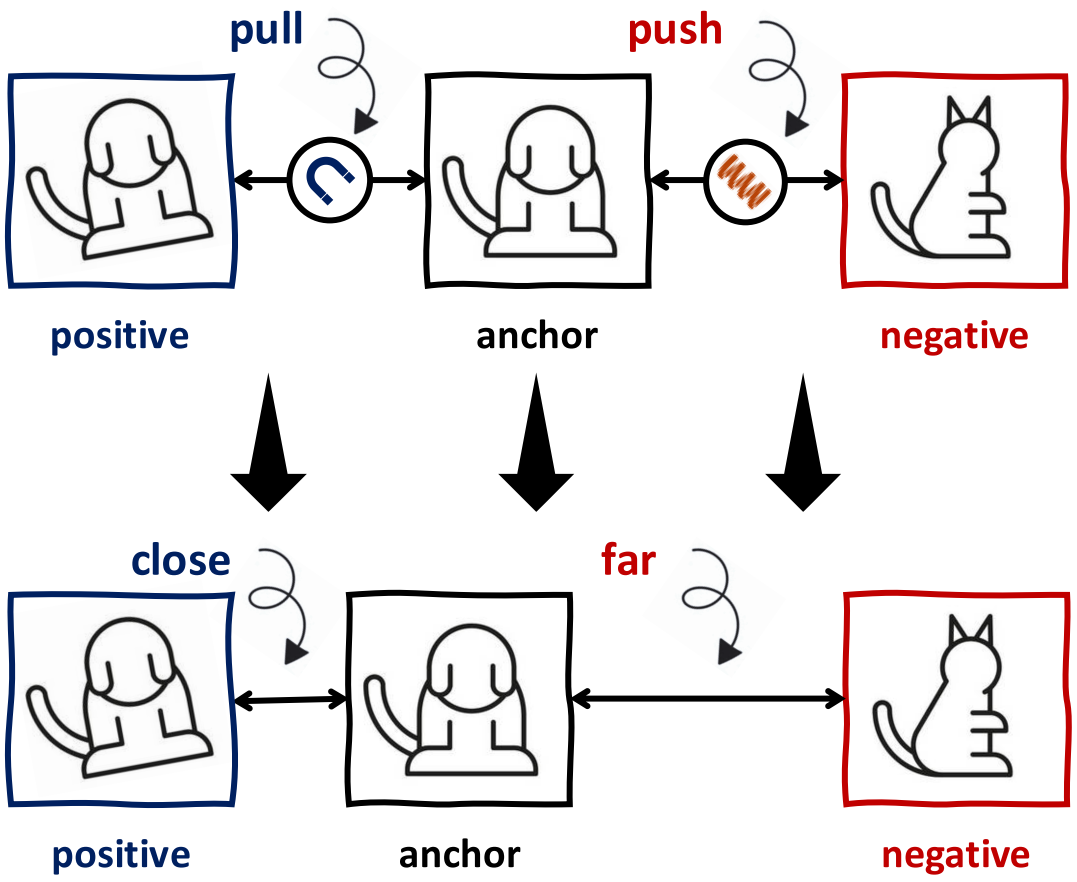
Pretext tasks

- ❖ **Contrastive Learning**: CSI, SSD
- ❖ **Reconstruction Learning**: MOOD
- ❖ **Pre-training**: CLIP

Representation: Contrastive Learning

Contrastive learning **improves the semantic structure of the embedding space** by **pulling** semantically similar samples together and **pushing** dissimilar ones apart.



Supervised Contrastive Learning

positive anchor

$$\mathcal{L}_{\text{con}}(x,\{x_+\},\{x_-\}) = -\frac{1}{|\{x_+\}|}\log\frac{\sum_{x'\in\boxed{\{x_+\}}}\exp\{\text{sim}(\boxed{z(x)},z(x'))\}}{\sum_{x'\in\{x_+\}\cup\boxed{\{x_-\}}}\exp\left(\text{sim}(z(x),z(x'))\right)}$$

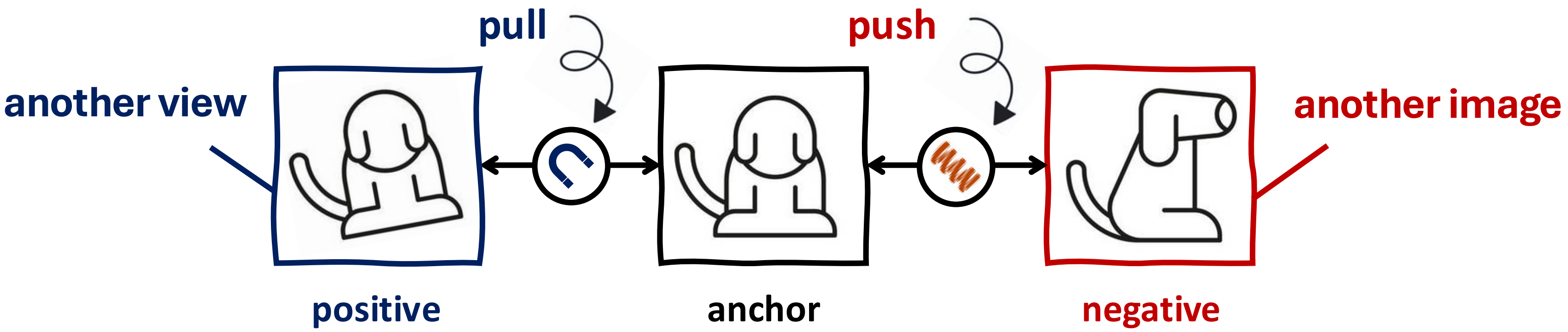
negative

Increasing similarity *between the anchor and* ***positive samples****, while* ***decreasing similarity*** *to* ***negative samples****.*

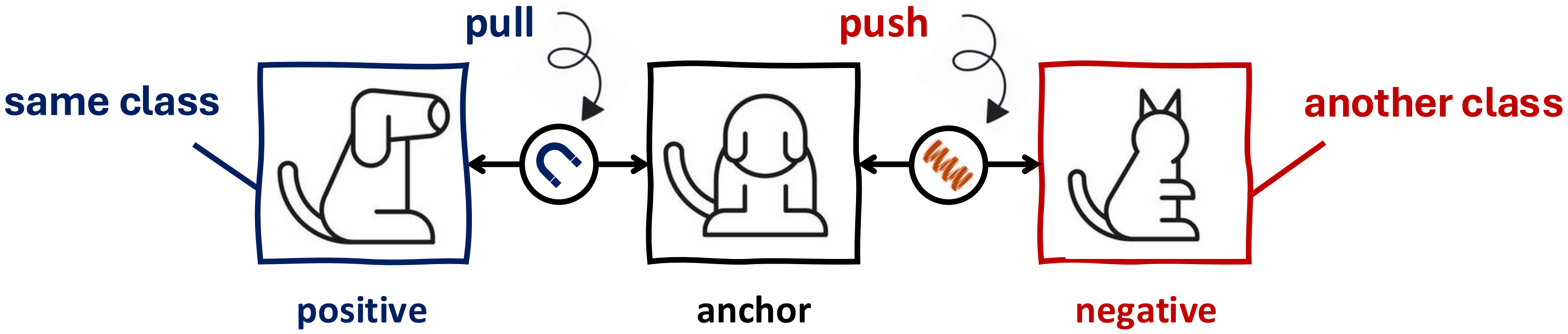
Representation: Contrastive Learning——SSD

SSD [a] Training Objective.

❖ **SSD**, discriminating between **individuals (label-agnostic)**.



❖ **SSD+**, discriminating between **classes (label-aware)**.



[a] Sehwag et al. SSD: A Unified Framework for Self-supervised Outlier Detection. In ICLR, 2021.

Representation: Contrastive Learning——SSD

SSD OOD Detector.

❖ **Mahalanobis**, cluster-conditioned detection **(OOD-agnostic)**.

k-th ID cluster centroid

$$s_{\mathrm{mah}}(x;\boldsymbol{\theta}) = \min_k (z(x)-\mu_k)^\top \boxed{\Sigma_k^{-1}}(z(x)-\boxed{\mu_k})$$

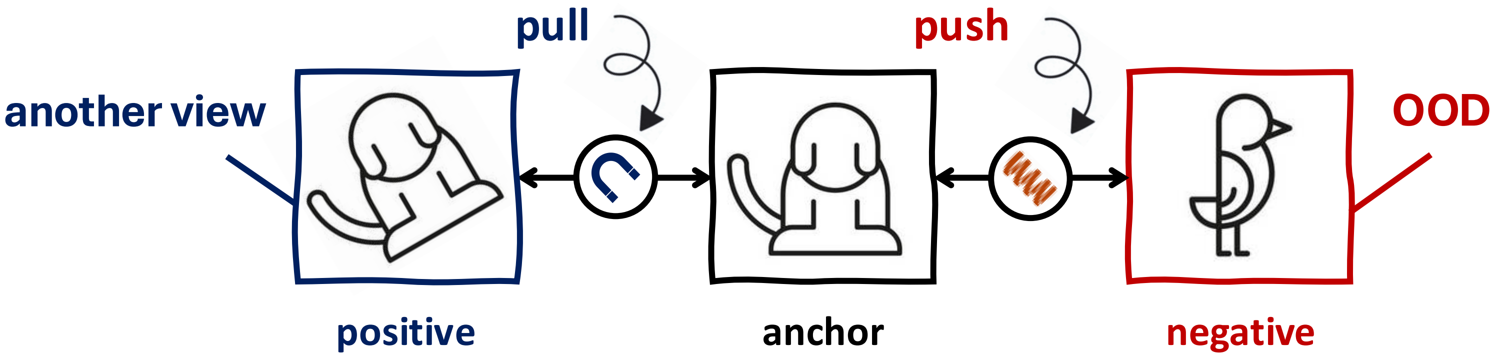
k-th ID cluster covariance, decorrelating features

❖ **Mahalanobis+**, a small OOD set is available before inference **(few-shot OOD)**.

$$s_{\mathrm{mah+}}(x;\boldsymbol{\theta}) = \underbrace{(z(x)-\mu_{id})^\top\Sigma_{id}^{-1}(z(x)-\mu_{id})}_{\textbf{distance to overall ID centroid}} - \underbrace{(z(x)-\mu_{ood})^\top\Sigma_{ood}^{-1}(z(x)-\mu_{ood})}_{\textbf{distance to overall OOD centroid}}$$

Representation: Contrastive Learning——CSI

CSI [a] further studies effective **negative transformation** to discriminate OOD samples.



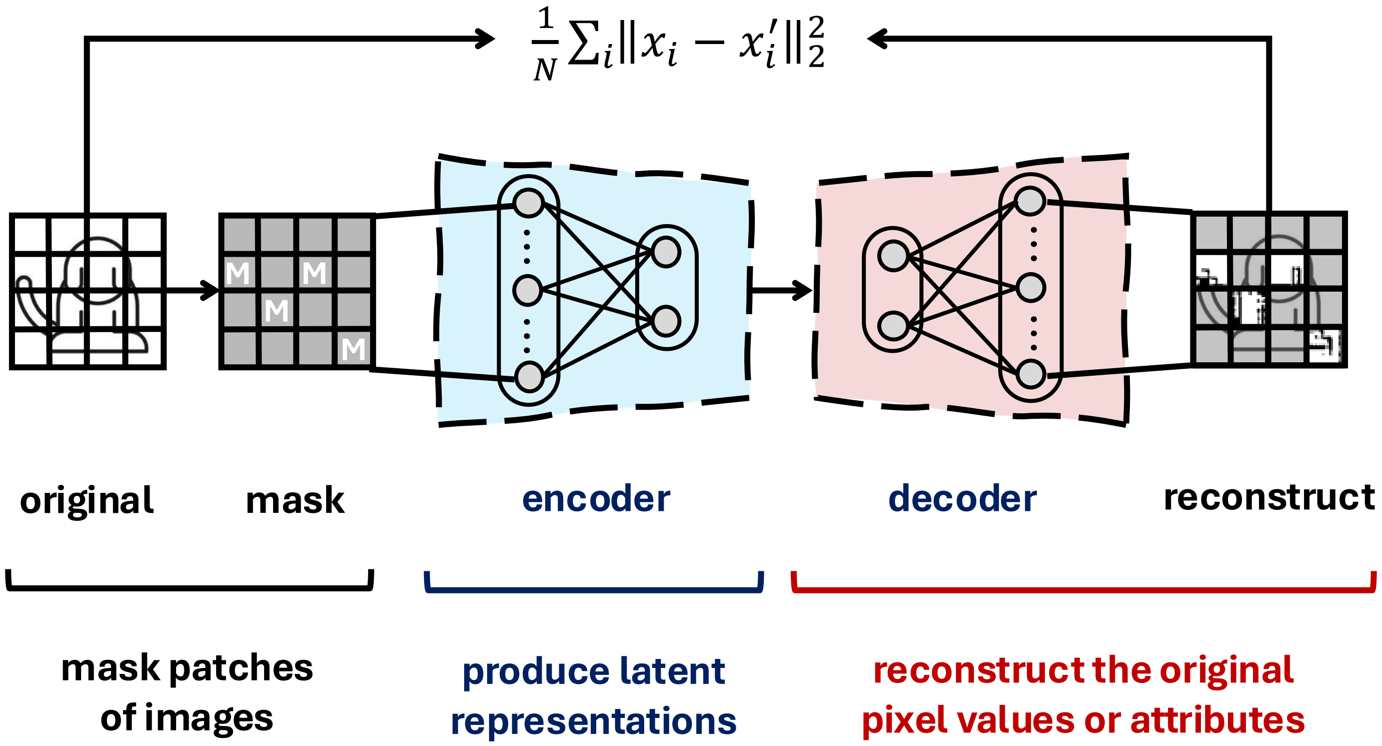
What if no OOD data are available? Those transformations previously found **ineffective as positive transformations** can instead be used as negative transformations.

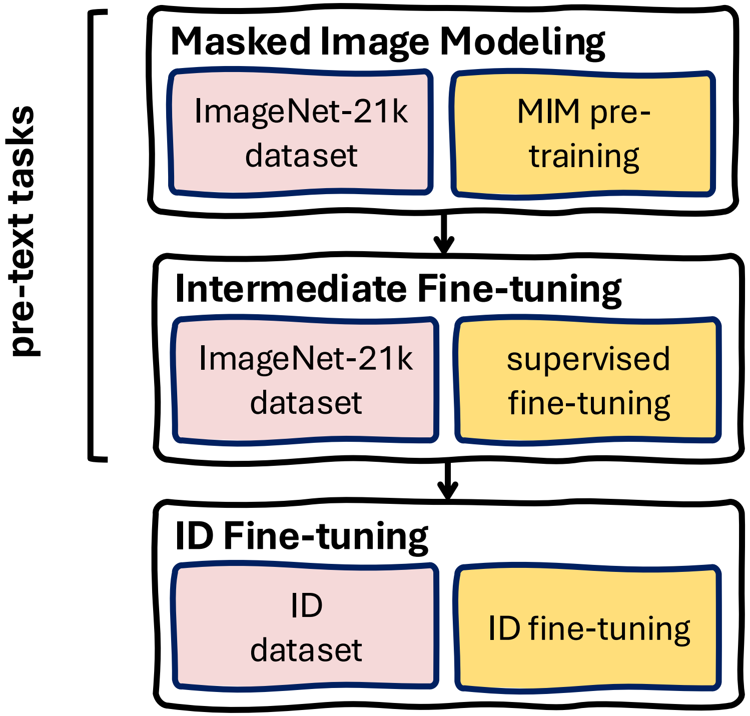
Figure from [a].

[a] Tack et al. CSI: Novelty Detection via Contrastive learning on Distributionally Shifted Instances. In NeurIPS, 2022.

Representation: Reconstruction Learning——MOOD

MOOD [a] forces the models to **encode finer-grained information needed to rebuild input**, which is far beyond semantics as in contrastive learning.

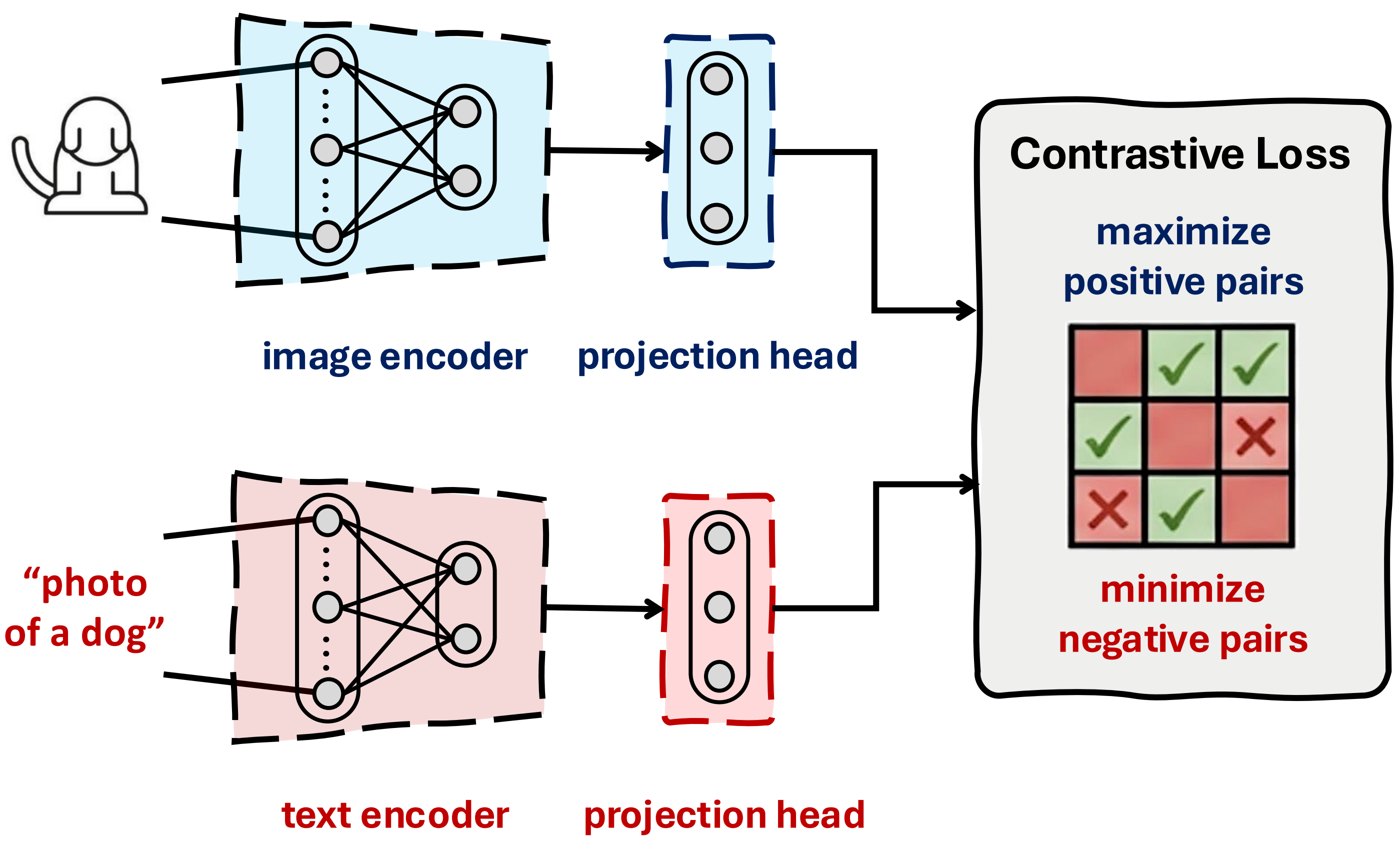


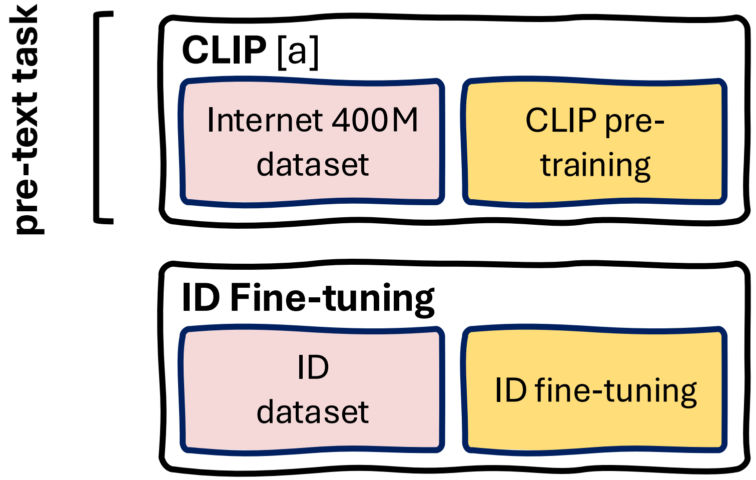


[a] Li et al. Rethinking Out-of-distribution (OOD) Detection: Masking Image Modeling is All You Need. In CVPR, 2023.

Representation: Pre-training——CLIP

Cross-modal alignment reduces reliance on **the shortcut to learn classification**, encouraging more general, semantically meaningful features.





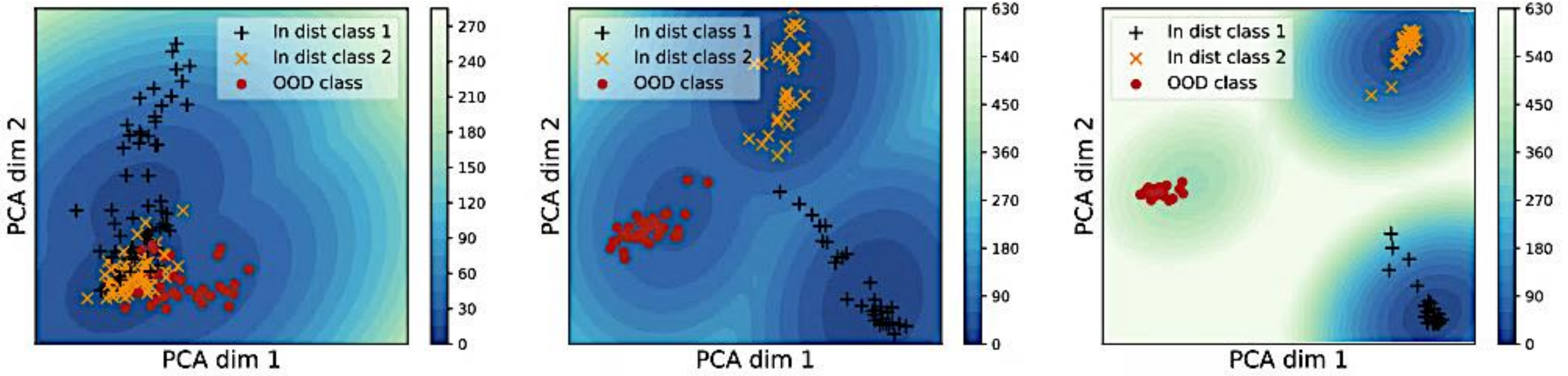
*Aligns **images and text representations** by **maximizing similarity of correct pairs**, meanwhile **minimizing similarity of incorrect pairs**.*

[a] Fort et al. Exploring the Limits of Out-of-Distribution Detection. In NeurIPS, 2021.

Representation: Pre-training——CLIP

Cross-modal alignment reduces reliance on **the shortcut to learn classification**, encouraging more general, semantically meaningful features.

ID training | CLIP pre-training | pre-training + fine-tuning



lower intra-class variance

higher inter-class variance

Figures of dimensional-reduced embeddings [a].

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Calibration: Overview

Let us review what we have learned from textbook [a].

❖ Maximum Likelihood & KL Divergence

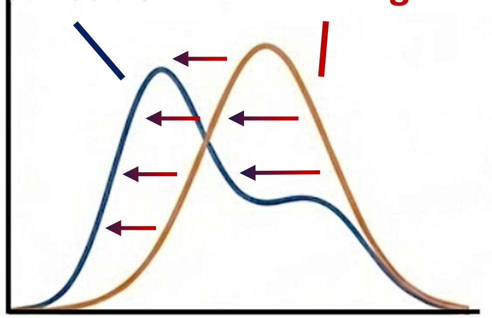
MLE minimizes KL between the **distribution model** and **empirical data distribution.**

optimal solution

$$p^* = \underbrace{\operatorname*{argmax}_{p \in \mathcal{P}} \sum_i \log p(x_i)}_{\text{Condition 1. proper distribution family}} = \underbrace{\operatorname*{argmin}_{p \in \mathcal{P}} \mathrm{KL}(\widehat{\mathcal{D}} || p)}_{\text{Condition 2. enough data}}$$

Condition 1.
proper distribution family

Condition 2.
enough data



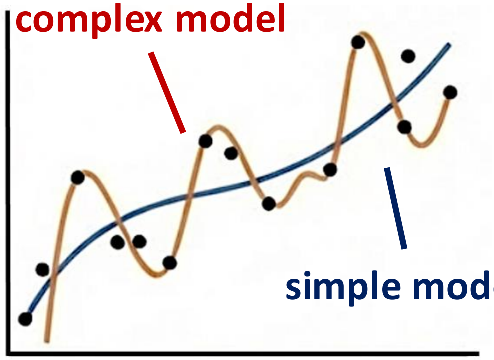
❖ Model Complexity & Estimation Error

Higher complexity increases estimation errors for a fixed dataset size.

estimation error

$$\left\| \mathbb{E}_{x \sim \mathcal{D}}[\Phi(x)] - \mathbb{E}_{x \sim \widehat{\mathcal{D}}}[\Phi(x)] \right\|_\infty \leq \underbrace{2\mathfrak{R}_m(\mathcal{H}) + r\sqrt{\frac{\log 2/\delta}{2m}}}_{\text{Condition 3. proper model family}}$$

Condition 3.
proper model family

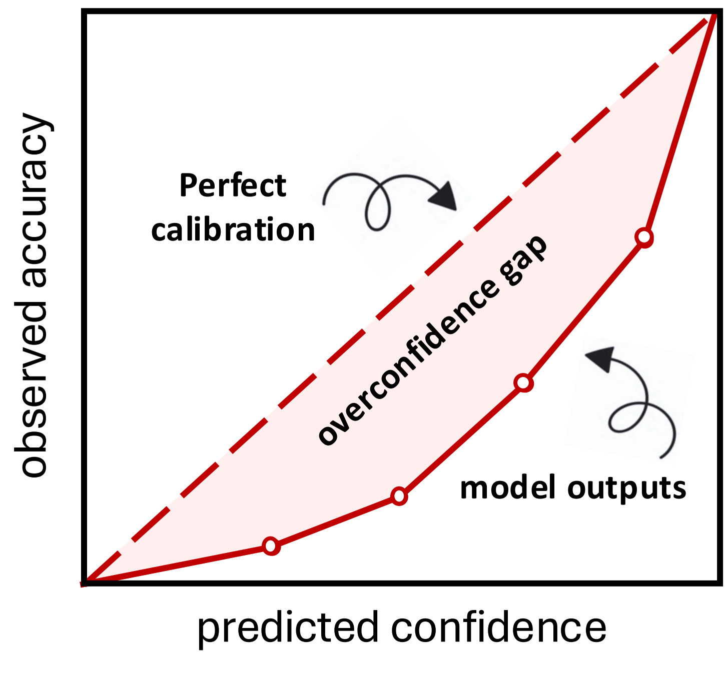


[a] Mohri et al. Foundations of Machine Learning. MIT press, 2018.

Calibration: Overview

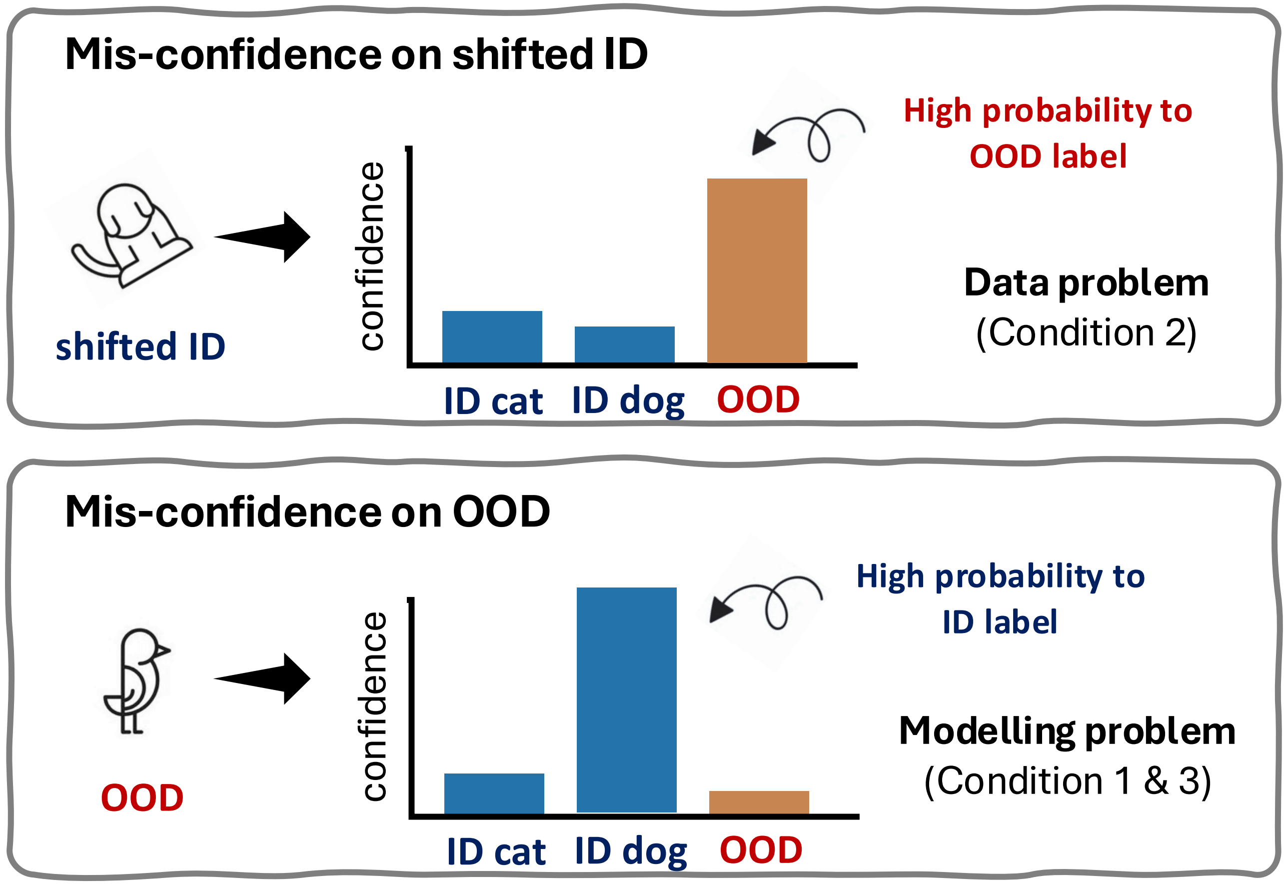
Conditions 1-3 may not be fully satisfied in practice, leading to calibration failures.

The overconfidence problem



Overconfidence makes the model outputs **appear more reliable than they really are.**

Consequences



Calibration: Overview

Conditions 1-3 may not be fully satisfied in practice, leading to calibration failures.

The overconfidence problem

❖ **Data-centric Solutions.**

conventional calibration methods, such as label smoothing and mixup augmentations.

❖ **Model-centric Solutions.**

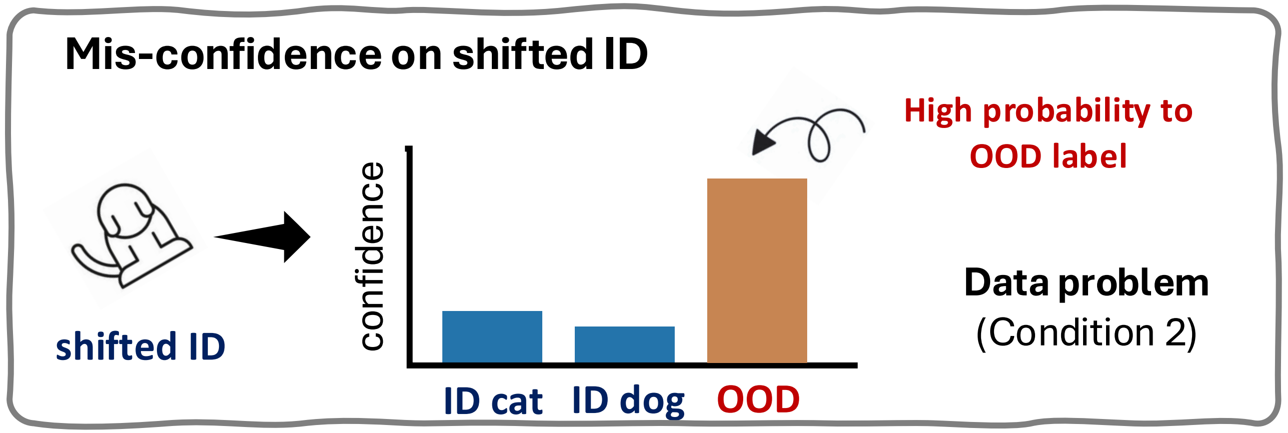
various **regularization strategies.**

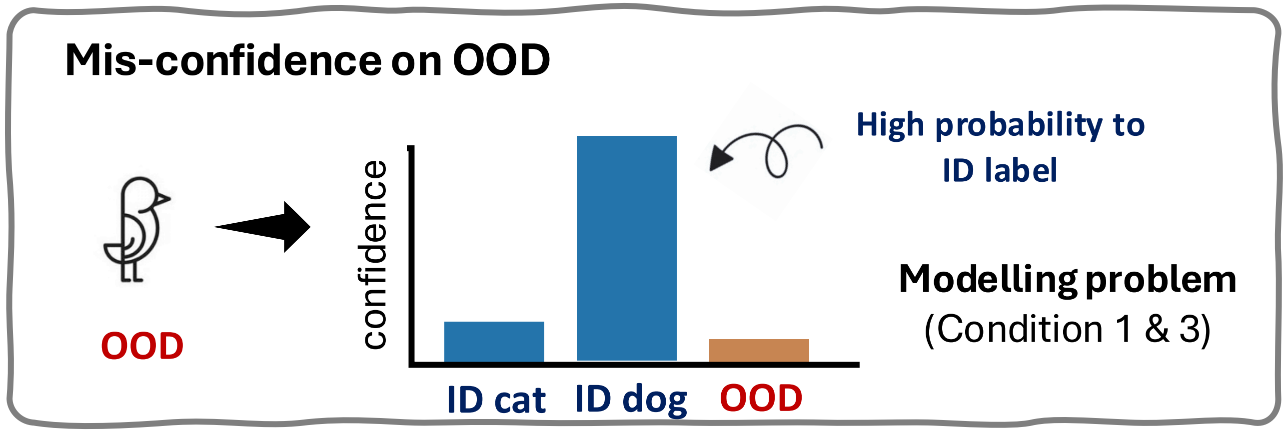
❖ **Distribution-centric Solutions.**

modelling **beyond softmax.**

Overconfidence makes the model outputs appear more reliable than they really are.

Consequences



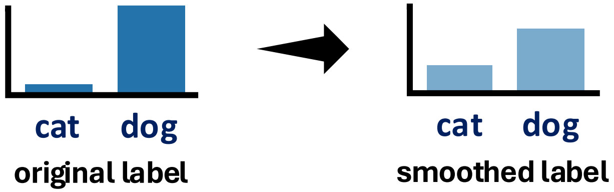


Calibration: Data-centric Solutions

Conventional calibration strategies have been empirically shown to enhance OOD detection.

❖ Change Labels

label smoothing [a]



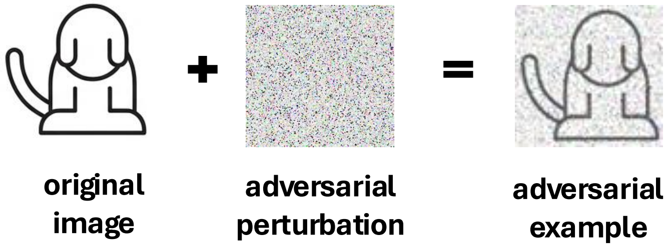
$$\tilde{y} = \overbrace{(1-\alpha)y + \frac{\alpha}{C}}^{\text{interpolation}}$$

original label uniform

replaces one-hot labels with **slightly softened targets.**

❖ Change Inputs

adversarial examples [b]



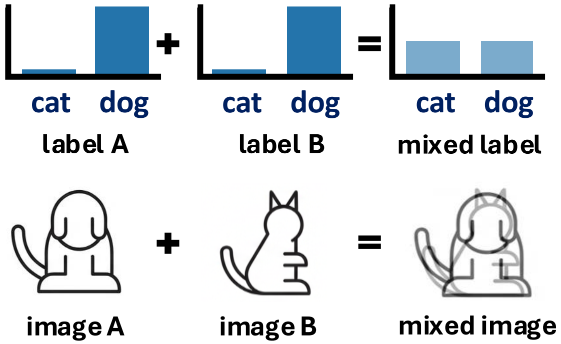
$$\underbrace{\max_{\delta \in \Delta}}_{\text{fail model}} \mathcal{L}(x+\delta, y, \theta)$$

fail model perturb input

perturbs inputs **imperceptibly** to fool the models and then train the model.

❖ Change Labels and Inputs

mixup [c]



$$\tilde{x} = \lambda x_A + (1-\lambda)x_B$$
$$\tilde{y} = \lambda y_A + (1-\lambda)y_B$$

creates virtual training examples that **interpolates** between data pairs.

[a] Li et al. Rethinking Out-of-distribution (OOD) Detection: Masked Image Modeling is All You Need. In CVPR, 2023.
[b] Botschen et al. Out-of-Distribution Detection with Adversarial Outlier Exposure. In CVPR, 2025.
[c] Zhang et al. *mixup*: Beyond Empirical Risk Minimization. In ICLR, 2018.

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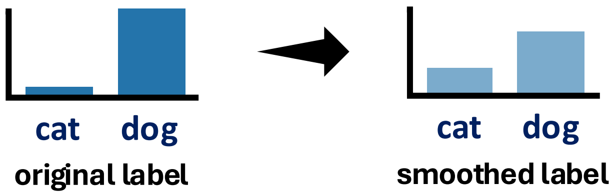

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original label uniform

replaces one-hot labels with **slightly softened targets.**

discourages extreme 0/1 probabilities and thus reduces overconfidence and improves calibrations.

❖ Change Inputs

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❖ Change Labels and Inputs

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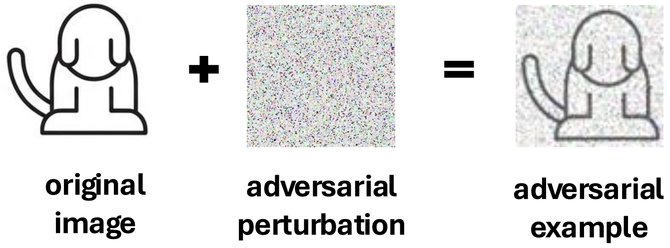

$$\underbrace{\max_{\delta\in\Delta}}_{\text{fail model}} \mathcal{L}(x + \delta, y, \theta)$$

fail model perturb input

perturbs inputs **imperceptibly** to fool the models and then train the model.

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mixup [c]

$$\tilde{x} = \lambda x_A + (1-\lambda)x_B$$

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encourages the model to **spread probability mass more cautiously** around decision boundaries.

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interpolation

$$\tilde{y} = (1-\alpha)y + \frac{\alpha}{c}$$

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replaces one-hot labels with **slightly softened targets.**

❖ Change Inputs

adversarial examples [b]

$$\max_{\delta \in A} \mathcal{L}(f(x+\delta), y; \theta)$$

fail model perturb input

perturbs inputs **imperceptibly** to fool the models and then train the model.

❖ Change Labels and Inputs

mixup [c]

$$\tilde{x} = \lambda x_{\mathrm{A}} + (1-\lambda) x_{\mathrm{B}}$$
$$\tilde{y} = \lambda y_{\mathrm{A}} + (1-\lambda) y_{\mathrm{B}}$$

interpolates empirical distribution into a continuous one via a convex combinations of data and labels.

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Calibration: Model-centric Solutions

Relationship between MSP and Free Energy

softmax prediction

$$P(Y = y|X) = \frac{\overbrace{\exp\{h_y(X)\}}^{\propto P(Y,X)}}{\underbrace{\sum_{y'} \exp\{h_{y'}(X)\}}_{\propto P(X)\text{, free energy}}}$$

Free energy, which models $P(X)$, is more reliable for OOD detection than maximum softmax prediction. **Why?**

A Bayesian View [a].

Considering the following two learning goals, **which one is more suitable for OOD detection?**

$$\underbrace{\mathbb{P}(y \neq \underbrace{\boxed{f(x)}}_{\text{classifier}}, r(x) = 0)}_{\text{Risk of accepting data that are misclassified}} + \underbrace{c_0 \mathbb{P}(\underbrace{\boxed{r(x)}}_{\text{rejector}} = 1)}_{\text{Risk of rejecting data with cost } c_0}$$

$$\underbrace{\alpha \underbrace{\boxed{\mathbb{P}_{\text{in}}}}_{\text{ID distribution}}(r(x) = 1)}_{\text{Risk of rejecting ID}} + \underbrace{\beta \underbrace{\boxed{\mathbb{P}_{\text{ood}}}}_{\text{OOD distribution}}(r(x) = 0)}_{\text{Risk of accepting OOD}}$$

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😭 $$\mathbb{P}(y \neq f(x), r(x) = 0) + c_0 \mathbb{P}(r(x) = 1)$$

used for **abstention-aware classification.**

$$r^*(x) = [\![\underbrace{\max_y \mathbb{P}(y|x)}_{\text{free energy}} < 1 - c_0]\!]$$

😃 $$\alpha \mathbb{P}_{\text{in}}(r(x) = 0) + \beta \mathbb{P}_{\text{ood}}(r(x) = 1)$$

used for **OOD detection.**

$$r^*(x) = \left[\!\!\left[\frac{\mathbb{P}_{\text{in}}(x)}{\mathbb{P}_{\text{ood}}(x)} < \frac{\beta}{\alpha} \right]\!\!\right] \approx \left[\!\!\left[\overbrace{\frac{\mathbb{P}_{\text{in}}(x)}{\tau}}^{\text{MSP}} < \frac{\beta}{\alpha} \right]\!\!\right]$$

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Free energy, which models $P(X)$, is more reliable for OOD detection than maximum softmax prediction. However, $P(X)$ is also not well-calibrated. So, **how to calibrate $P(X)$?**

Calibrating $P(Y)$ (low dimension) offers a sufficient condition of **calibrating $P(X)$ (high dimension).**

Mathematical

$P(Y=y) = \frac{1}{Z}\int \exp\{h_y(x)\}dvx,$

where $Z = \sum_y \int \exp\{h_y(x)\}dvx$

→ **Monte Carlo**

Empirical

$\hat{P}(Y=y) = n_y/N$

→ **Count**

Hypothesis Test

$H_0: P(Y=y) = \hat{P}(Y=y)$

versus

$H_1: P(Y=y) \neq \hat{P}(Y=y)$

[a] Huang et al. Density-driven Regularization for Out-of-distribution Detection. In NeurIPS, 2022.

Calibration: Model-centric Solutions——DCR [a]

Relationship between MSP and Free Energy

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softmax prediction

$\propto P(Y,X)$

$\propto P(X)$, free energy

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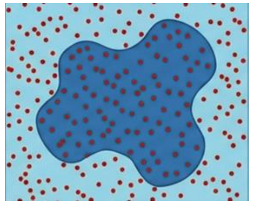

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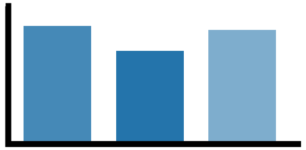
→ **Count**



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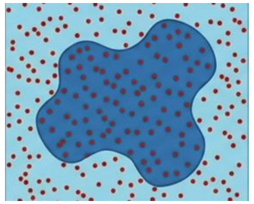

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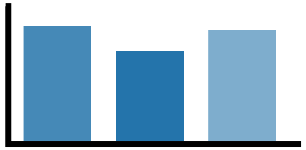

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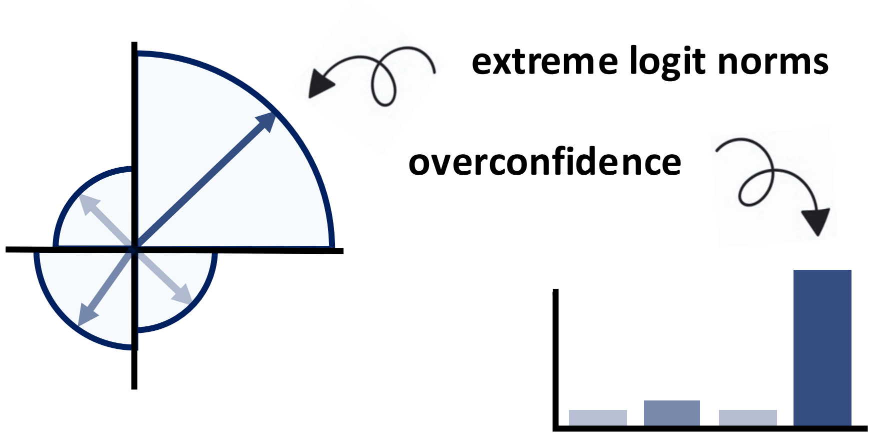
Calibration: Distribution-centric Solutions——LogitNorm

We seek **distribution modelling beyond Softmax** that are more proper for OOD detection.

Why is Softmax not sufficient?

- **Scaling logits** increases confidence and decreases the risk.
- **Training pushes near-zero risk**, driving large confidence and inflating logits.



Logit Norm [a]

- **normalizes logit vector** to a constant norm during training, following

$$-\log \frac{\exp\{f_y/(\tau\|f_y\|)\}}{\sum_i \exp\{f_i/(\tau\|f_i\|)\}}$$

normalization

[a] Wei et al. Mitigating Neural Network Overconfidence with Logit Normalization. In ICML, 2022.

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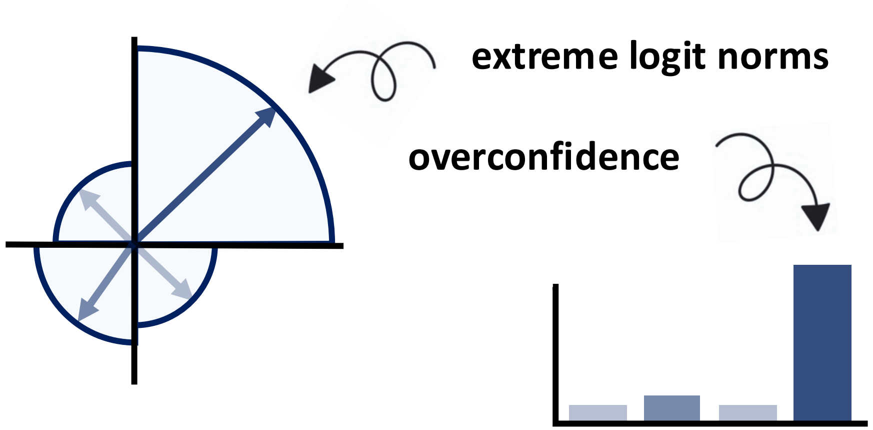

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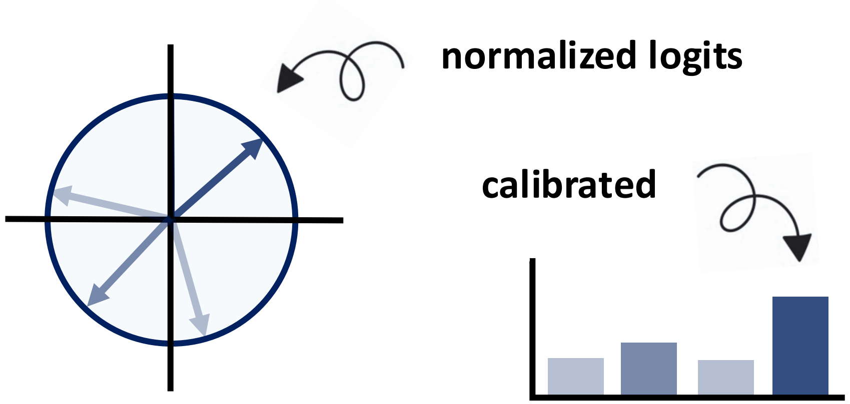

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- **The separation is piecewise linear** in feature space.
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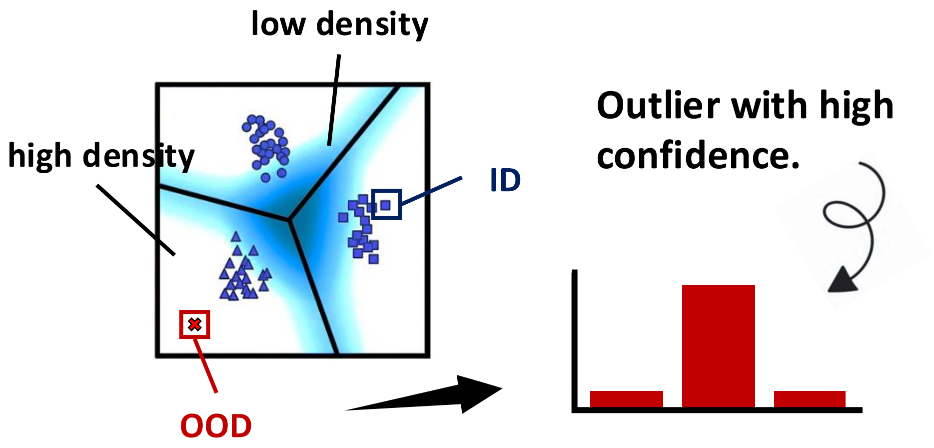

SIREN [a]

- The density depends on **similarity to prototypes** and vMF likelihood, creating a **curved, cluster-shaped** regions.

$$P(Y = c|r) \propto \exp\{\underbrace{\kappa_c}_{\text{concentration}} \underbrace{\mu_c^{\top}}_{\text{prototype}} r\}$$

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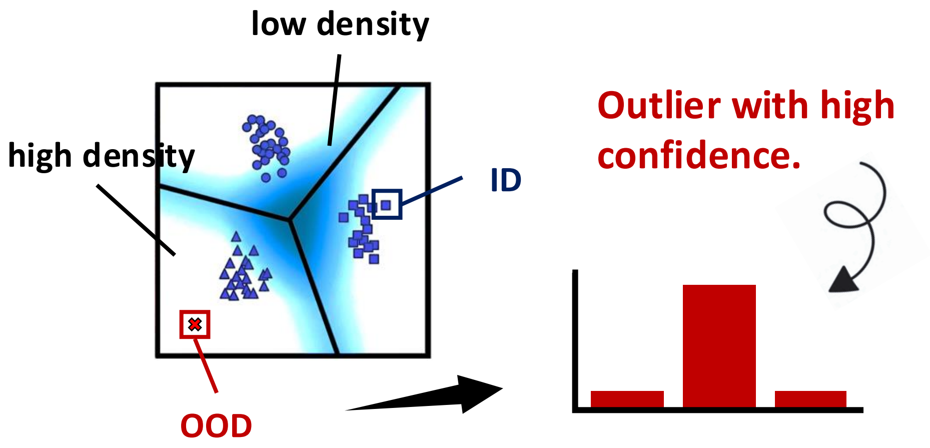

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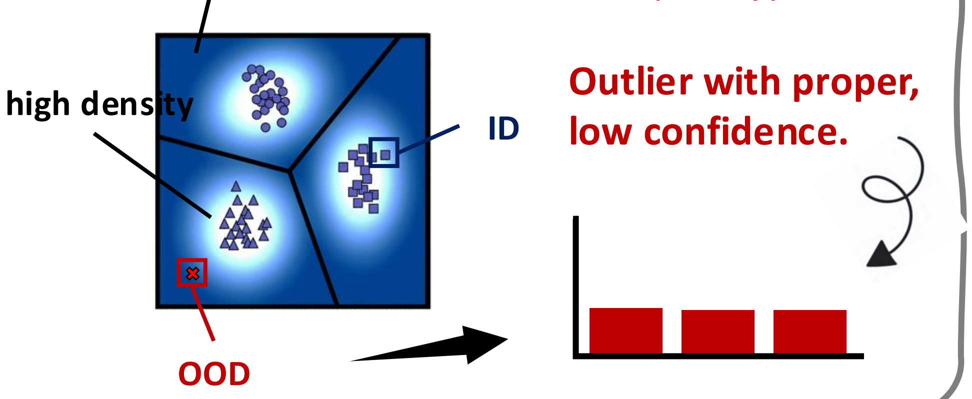

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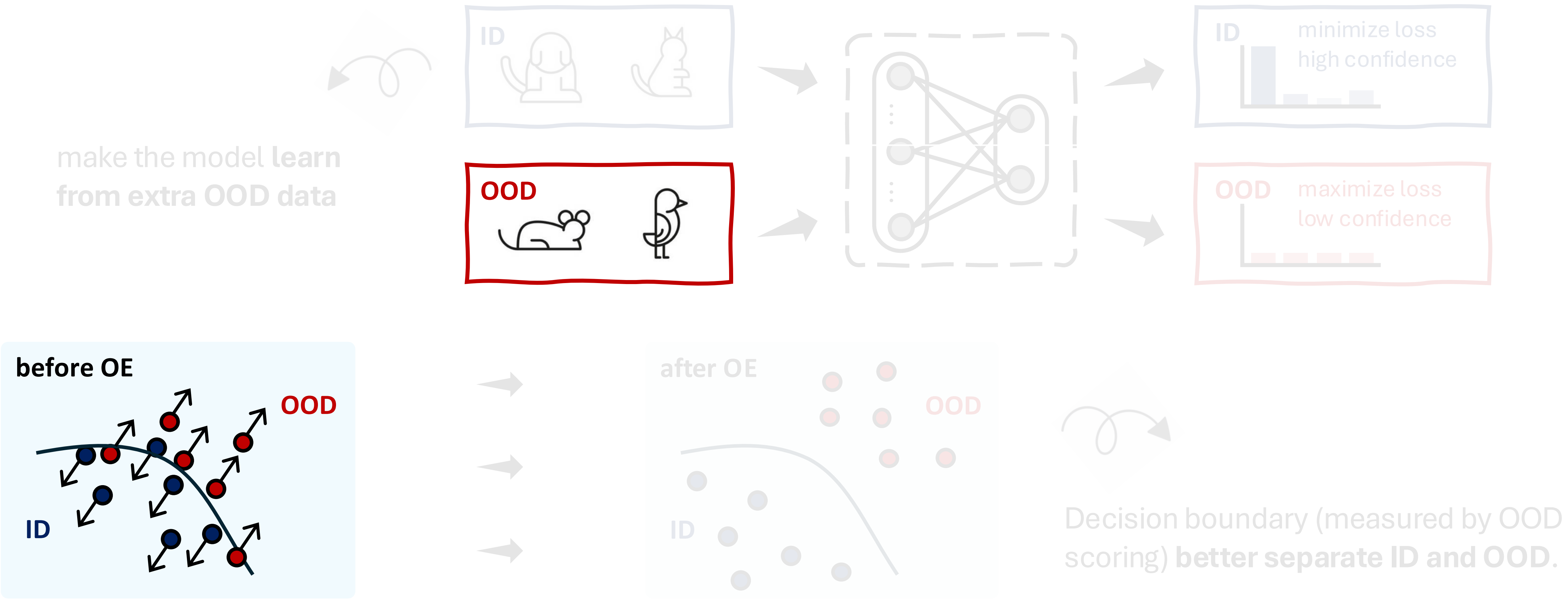
Outlier Exposure: Overview

Outlier exposure [a] takes OOD detection as **an additional binary classification task**, enabling models to directly learn to distinguish ID from OOD patterns.



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Outlier Exposure: Overview

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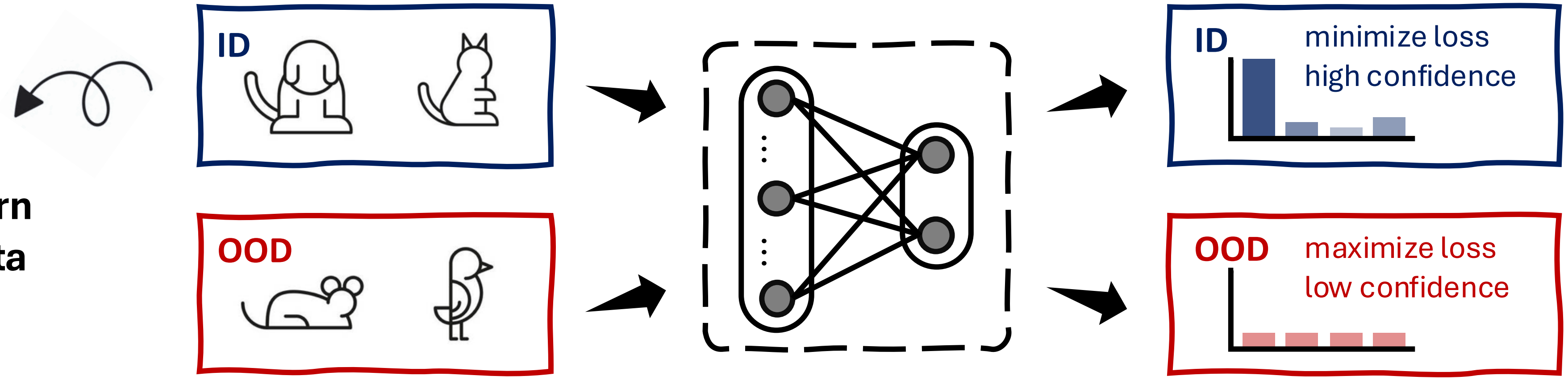
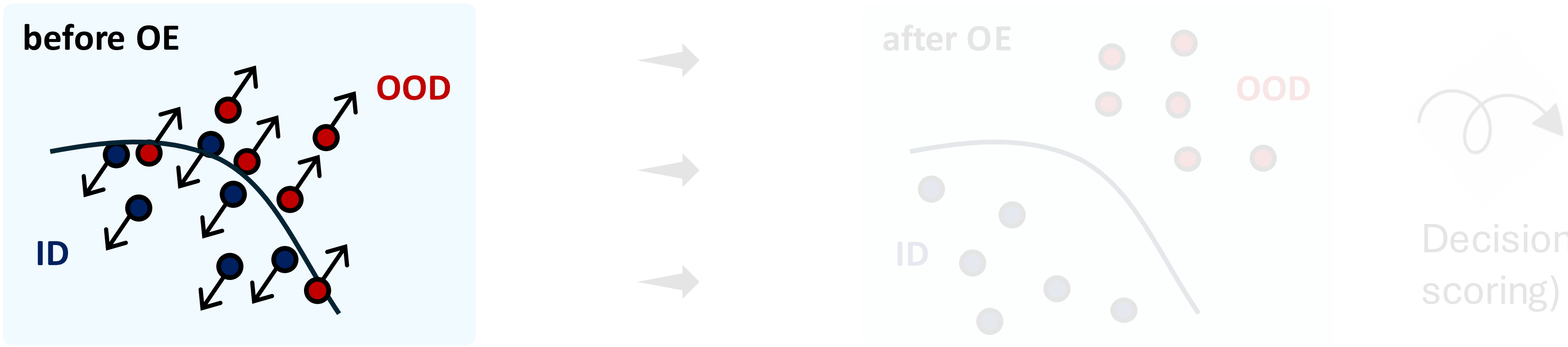
make the model **learn from extra OOD data**





Decision boundary (measured by OOD scoring) **better separate ID and OOD.**

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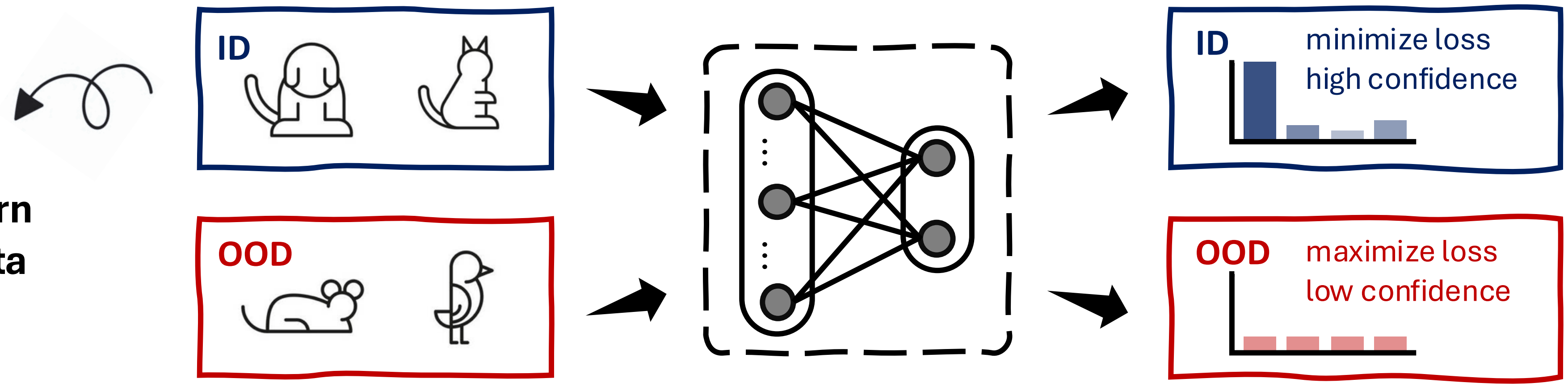

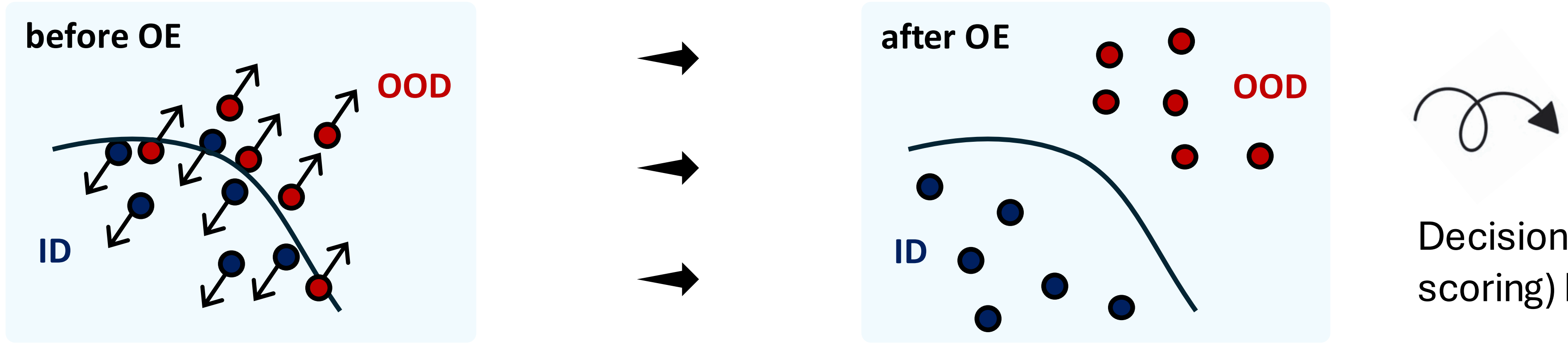

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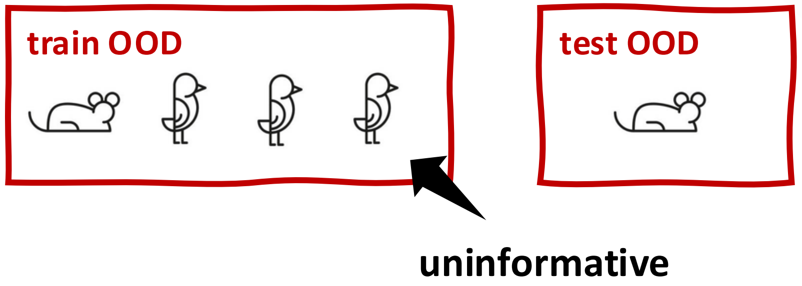
Outlier Exposure: Overview

Training and test OOD can differ, and **such distribution gap degrades OOD performance** [a].

❖ **Case 1.**

Redundant Data



Training data include test data,
but many samples are uninformative.

How to address Case 1?

Data sampling / reweighting to remove those uninformative samples.

❖ **Case 2.**

Scarce Data

Training data contains no test data.

How to address Case 2?

Data augmentation to enlarge the OOD coverage during training.

[a] Wang et al. Learning to Augment Distributions for Out-of-distribution Detection. In NeurIPS, 2023.

Outlier Exposure: Overview

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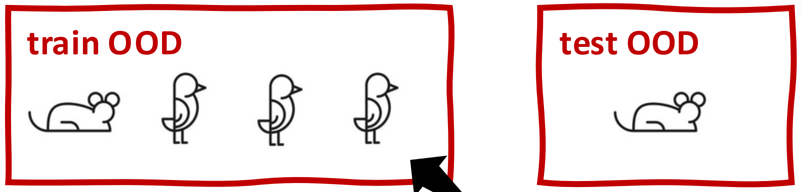
❖ **Case 1.**

Redundant Data



uninformative

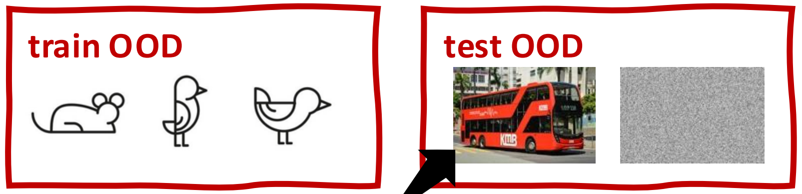
Training data include test data,
but many samples are uninformative.

How to address Case 1?

Data sampling / reweighting to remove those uninformative samples.

❖ **Case 2.**

Scarce Data



different pattern and semantics

Training data contains no test data.

How to address Case 2?

Data augmentation to enlarge the OOD coverage during training.

[a] Wang et al. Learning to Augment Distributions for Out-of-distribution Detection. In NeurIPS, 2023.

Outlier Exposure: Overview

Training and test OOD can differ, and **such distribution gap degrades OOD performance** [a].

❖ **Case 1.**

Redundant Data

train OOD

test OOD

uninformative

Training data include test data,
but many samples are uninformative.

How to address Case 1?

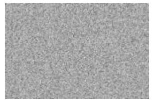
Data sampling / reweighting to remove those uninformative samples.

❖ **Case 2.**

Scarce Data

train OOD

test OOD



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Data augmentation to enlarge the OOD coverage during training.

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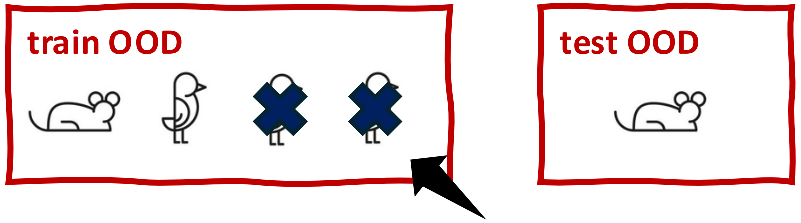
Outlier Exposure: Overview

Data sampling learns from fewer examples and **data augmentation from more**.

❖ **Case 1.**

Redundant Data → Data Sampling



learn from less data

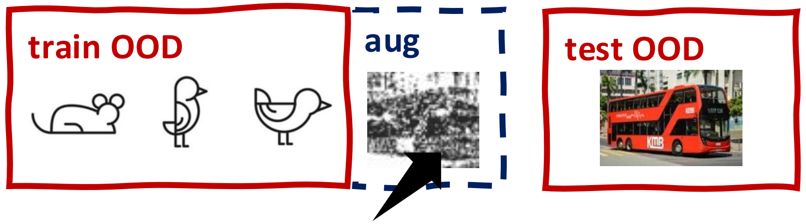
$$\mathbb{E}_{x\sim\mathcal{D}_{ood}}[\boxed{w_x}\ell_{ood}(x;\boldsymbol{\theta})]$$

reweighting

learn from resampled data

❖ **Case 2.**

Scarce Data → Data Augmentation



learn from extra data

$$\mathbb{E}_{x\sim\mathcal{D}_{ood}}[\ell_{ood}(x';\boldsymbol{\theta})],\ x' = \boxed{\Phi(x)}$$

augmentation

learn from extra data

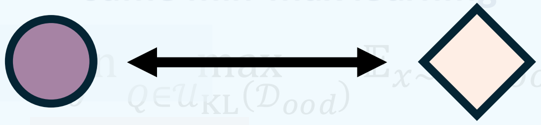
[a] Wang et al. Learning to Augment Distributions for Out-of-distribution Detection. In NeurIPS, 2023.

Outlier Exposure: Overview

Data sampling and augmentation **both improve distribution robustness** [a].

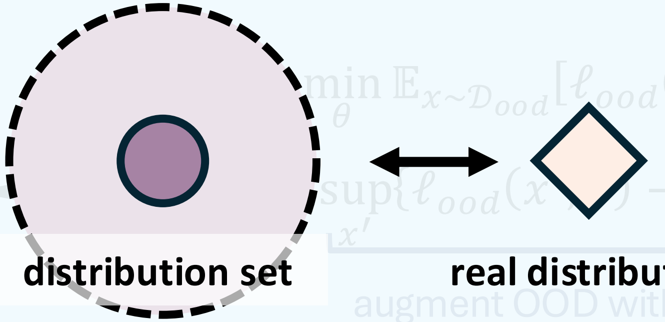
original distribution gap, $\min_{\theta} \mathbb{E}_{x\sim\mathcal{D}_{ood}}[\ell_{ood}(x;\boldsymbol{\theta})]$

The distribution gap degrade model performance.



augmented distribution gap, $\min_{\theta} \boxed{\max_{Q\in\mathcal{U}(\mathcal{D}_{ood})}} \mathbb{E}_{x\sim Q}[\ell_{ood}(x;\boldsymbol{\theta})]$

The model performs well for all distribution within the set.



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Outlier Exposure: Overview

Data sampling and augmentation **both improve distribution robustness** [a].

❖ **Case 1.**

Redundant Data → Data Sampling

same min-max learning

$$\min_{\theta} \max_{Q \in \mathcal{U}_{\mathrm{KL}}(\mathcal{D}_{ood})} \mathbb{E}_{x\sim Q}[\ell_{ood}(x;\boldsymbol{\theta})]$$

$$\mathcal{U}_{\mathrm{KL}}(\mathcal{D}_{ood}) \coloneqq \{Q: \mathrm{KL}(Q \| \mathcal{D}_{ood}) \leq \rho\}$$

different distribution set

$$\min_{\theta} \mathbb{E}_{x\sim\mathcal{D}_{ood}}[w_x \ell_{ood}(x;\theta)]$$

$$w_x = \underbrace{\frac{\exp\{\ell_{ood}(x;\theta)\ /\eta\}}{\int \exp\{\ell_{ood}(x;\theta)\ /\eta\}dx}}_{\text{up-weight OOD with larger loss}}$$

❖ **Case 2.**

Scarce Data → Data Augmentation

same min-max learning

$$\min_{\theta} \max_{Q \in \mathcal{U}_{\mathrm{W}}(\mathcal{D}_{ood})} \mathbb{E}_{x\sim Q}[\ell_{ood}(x;\boldsymbol{\theta})]$$

$$\mathcal{U}_{\mathrm{W}}(\mathcal{D}_{ood}) \coloneqq \{Q: \mathrm{Wass}(Q, \mathcal{D}_{ood}) \leq \rho\}$$

different distribution set

$$\min_{\theta} \mathbb{E}_{x\sim\mathcal{D}_{ood}}[\ell_{ood}(x';\theta)]$$

$$x' = \underbrace{\sup_{x'}\{\ell_{ood}(x';\theta) - \gamma\|x', x\|_2\}}_{\text{augment OOD with larger loss}}$$

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Data sampling and augmentation **both improve distribution robustness** [a].

- **Case 1.**

Redundant Data → Data Sampling

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up-weight OOD with larger loss

- **Case 2.**

Scarce Data → Data Augmentation

same min-max learning

$$\min_{\theta} \max_{Q \in \mathcal{U}_{\mathrm{W}}(\mathcal{D}_{ood})} \mathbb{E}_{x \sim Q}[\ell_{ood}(x; \boldsymbol{\theta})]$$

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augment OOD with larger loss

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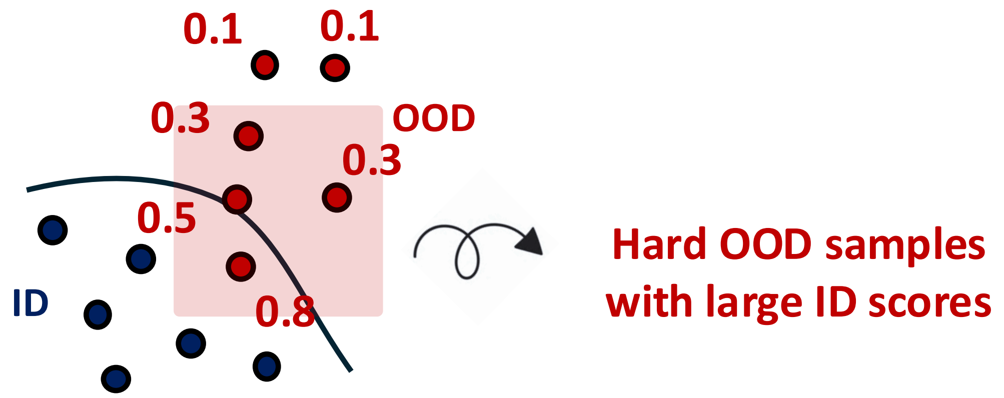
Outlier Exposure: Sampling

ATOM [a]

- **Hard OOD data** should be sampled more during training.
- **Large ID scores on OOD samples** indicates hard OOD data.



POEM [b]

- OOD data **near the ID/OOD boundary** should be sampled more.
- Bayesian classifiers capture parameter uncertainty, **improving exploration.**

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[b] Ming et al. POEM: Out-of-distribution Detection with Posterior Sampling. In ICML, 2022.

Outlier Exposure: Sampling

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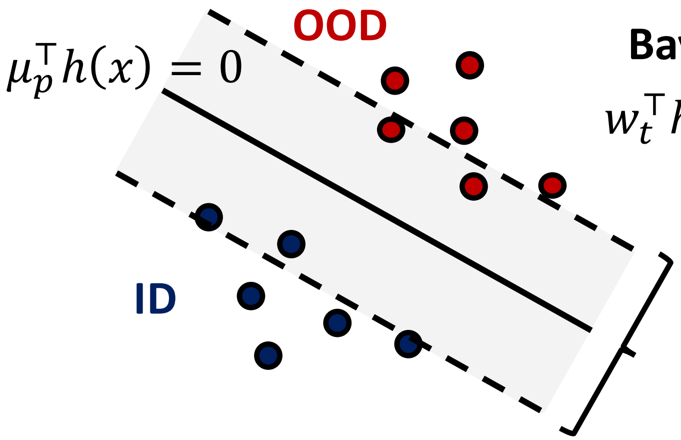

Bayesian ID/OOD classifier

$w_t^\top h(x) = 0, w_t \sim \mathcal{N}(\mu_p, \Sigma_p)$

High Variance in w_t, measured by Σ_p.

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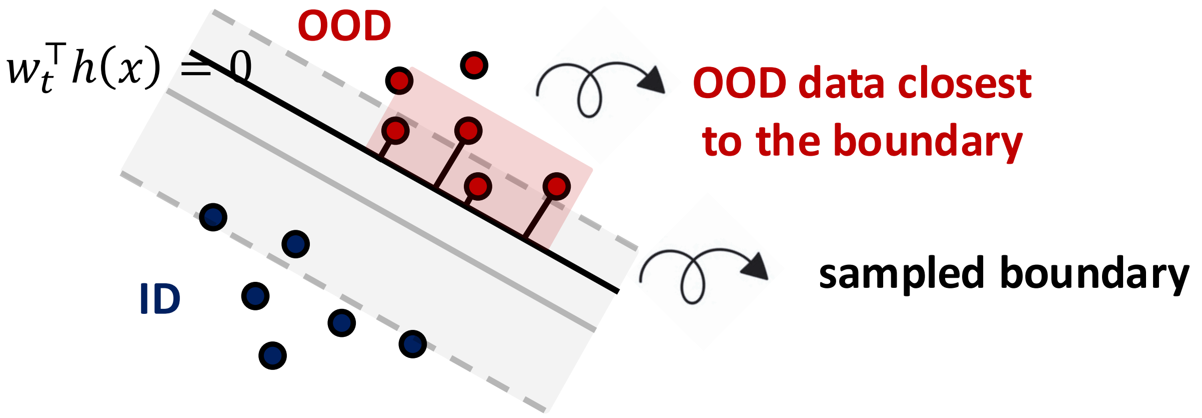

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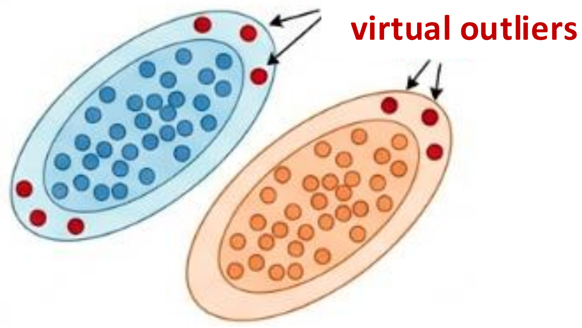
Outlier Exposure: Augmentation

Augmentation can be conducted in either **embedding space** or input space.

❖ Synthesis

VOS [a]

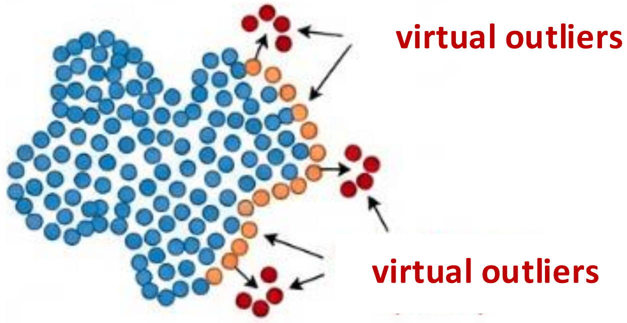
class-conditional **Gaussian modelling**



- ❖ estimate μ and Σ per class.
- ❖ sample $v \sim \mathcal{N}(\mu_c, \Sigma)$.
- ❖ keep only low likelihood samples with $p(v) < \epsilon$.

NPOS [b]

Non-parametric K-NN modelling



- ❖ Identify boundary ID with high k-NN.
- ❖ sample locally around boundary $v \sim \mathcal{N}(h_{bdy}, \sigma^2 I)$.
- ❖ keep candidates with large k-NN.

❖ Augmentation

DAL [c]

worst-case **OOD augmentation**

- ❖ sample original OOD data.
- ❖ gradient ascent to increase their respective loss values.
- ❖ augmented OOD data for training.

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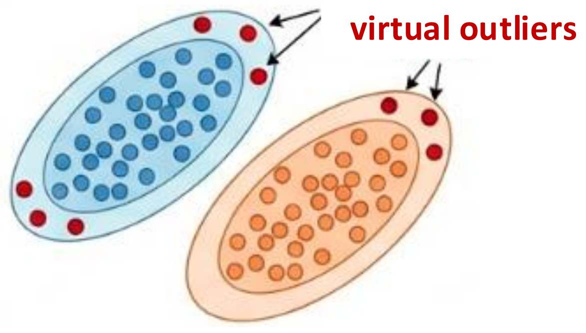

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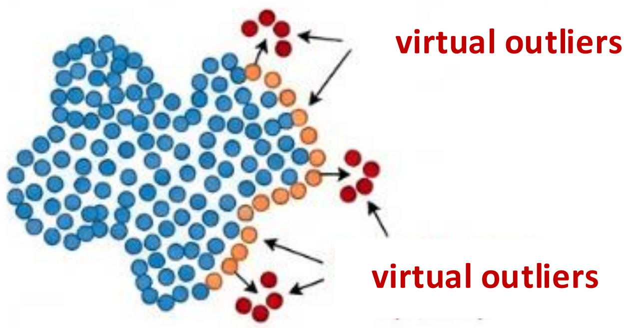

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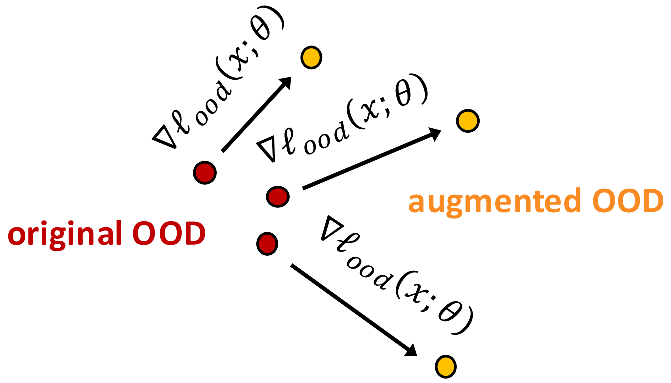

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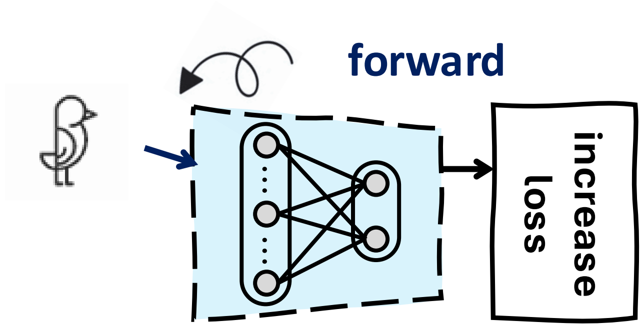
Outlier Exposure: Augmentation

Augmentation can be conducted in either embedding space or **input space**.

❖ Adversarial Training [a]



perturb inputs to maximize OOD loss values, thus creating worst-case examples.

❖ Generative Model [b]

perturb latent embedding to maximize OOD loss values, thus creating worst-case examples.

❖ Implicit Synthesis [c]

$$\underbrace{[W(I+\alpha A)]^{\top} x}_{\text{model perturb}} = \underbrace{W^{\top}[x+\alpha A^{\top} x]}_{\text{feature perturb}}$$

perturb parameters that maximize OOD loss can implicitly create worst-case examples.

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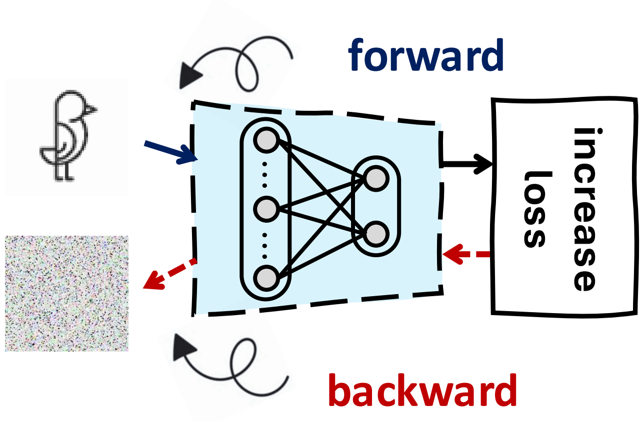

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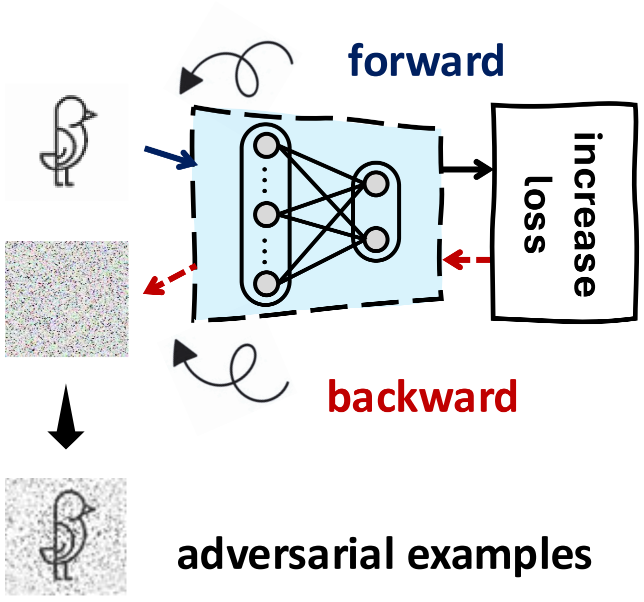

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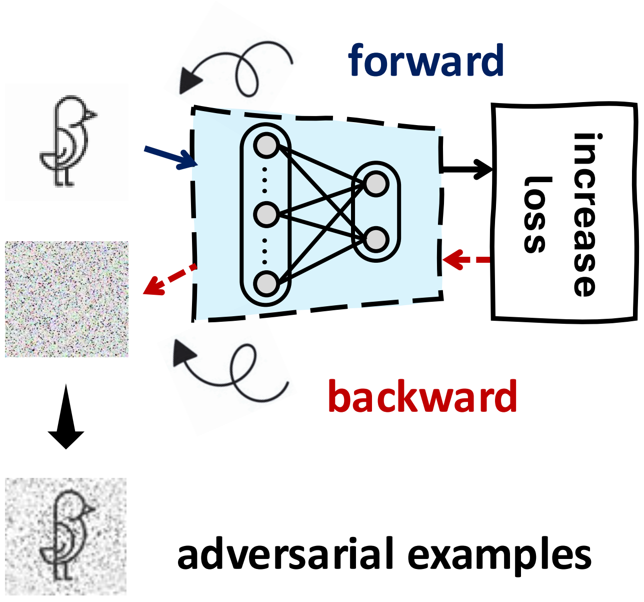

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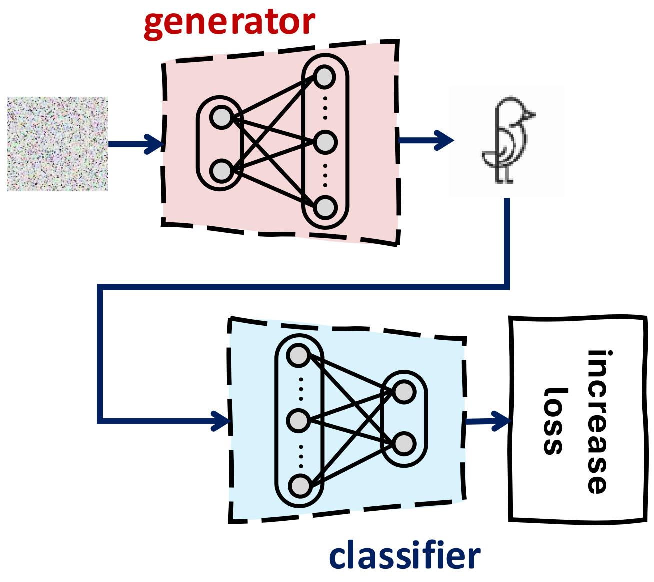

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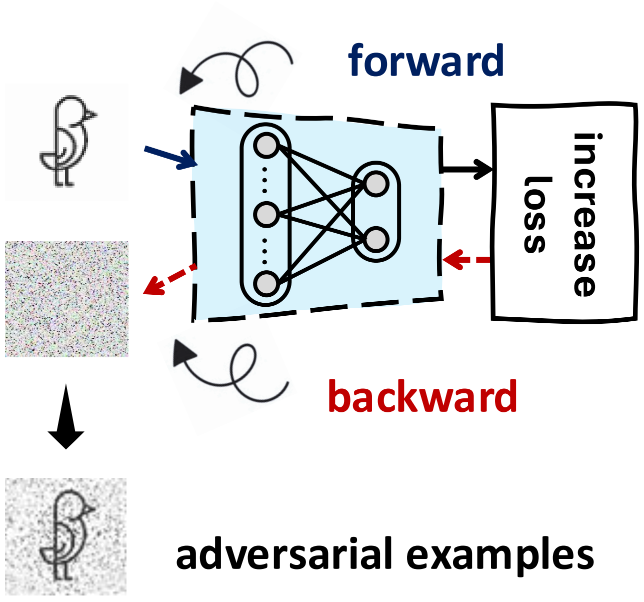

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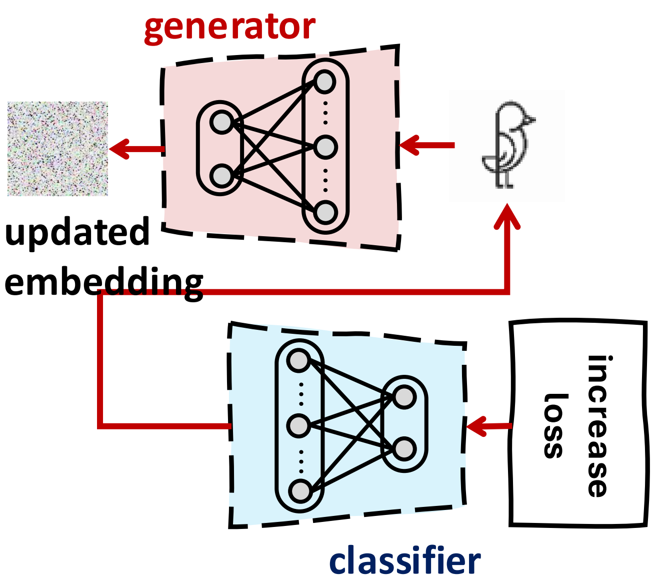

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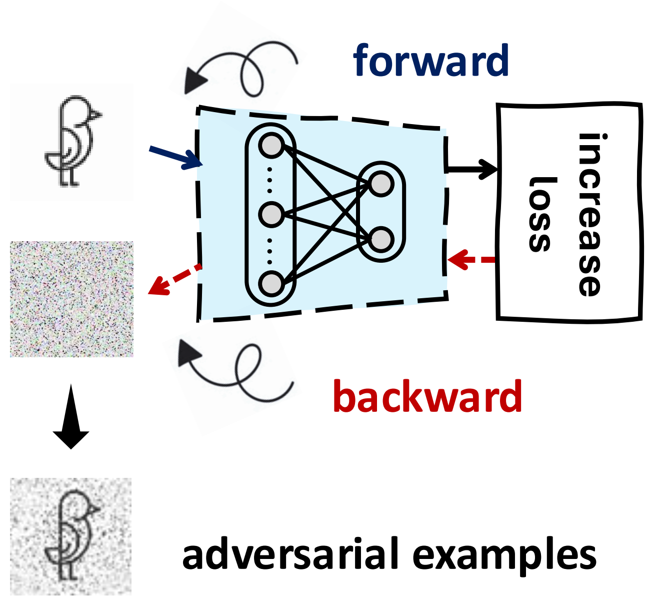

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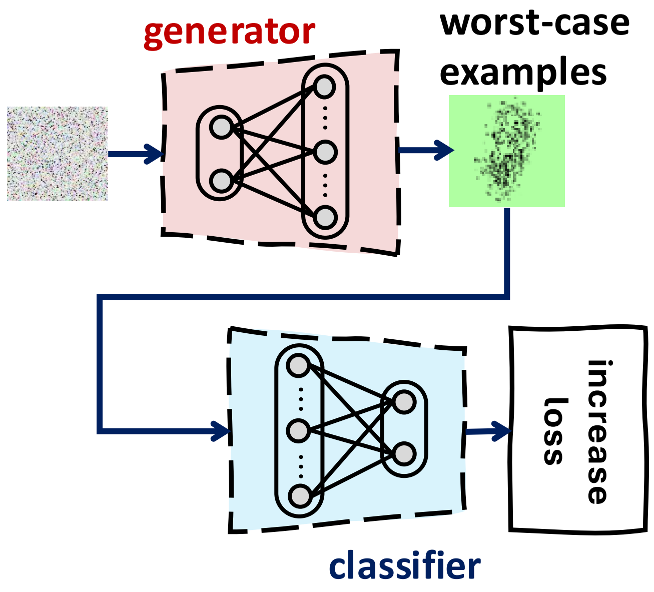

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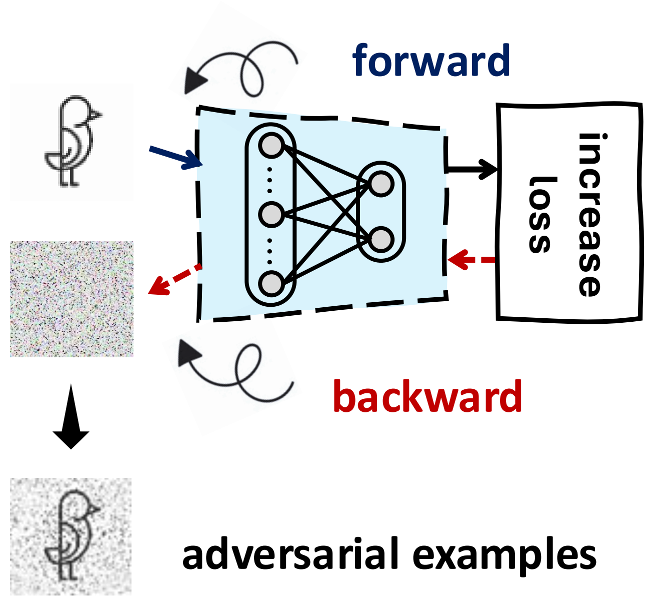

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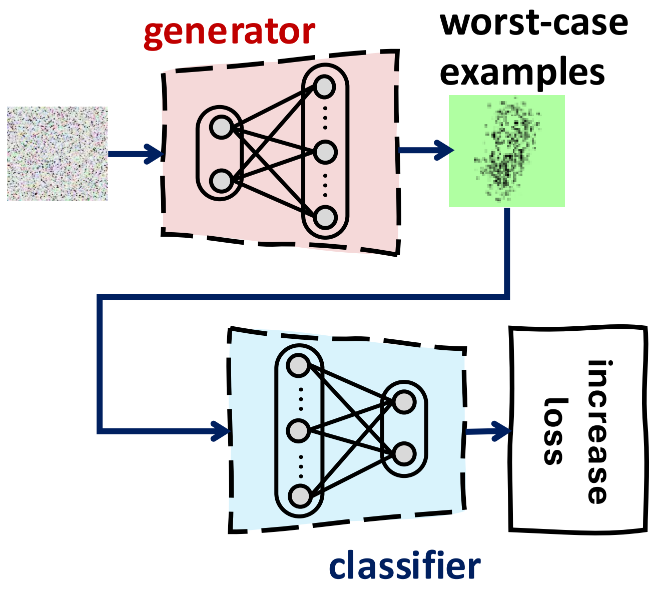

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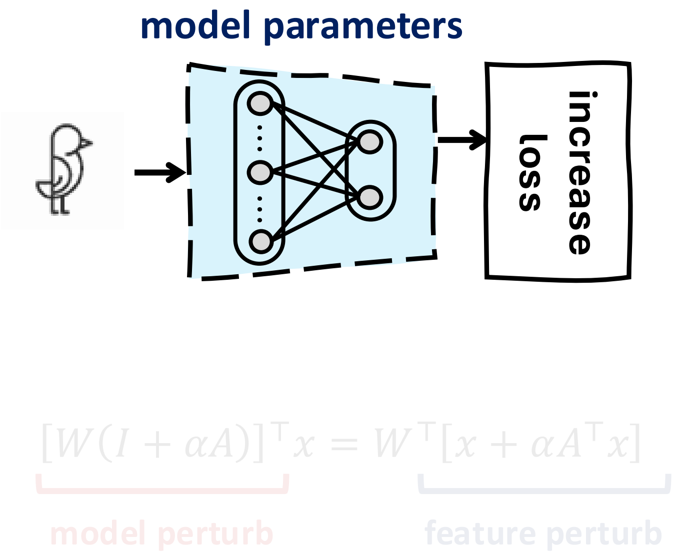

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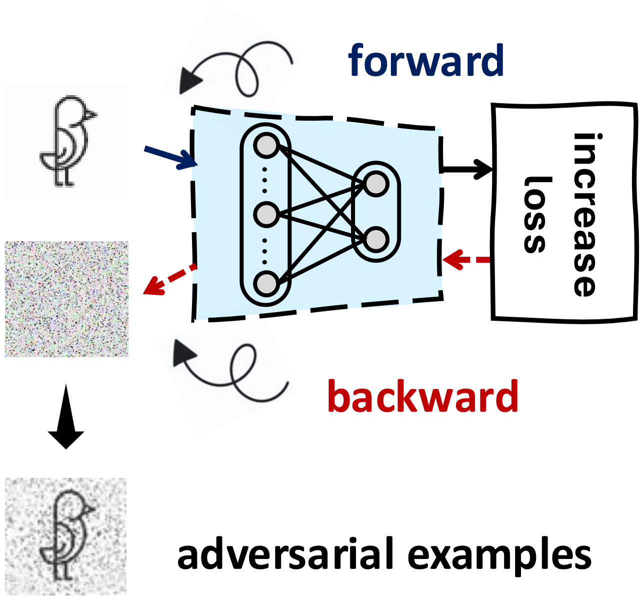

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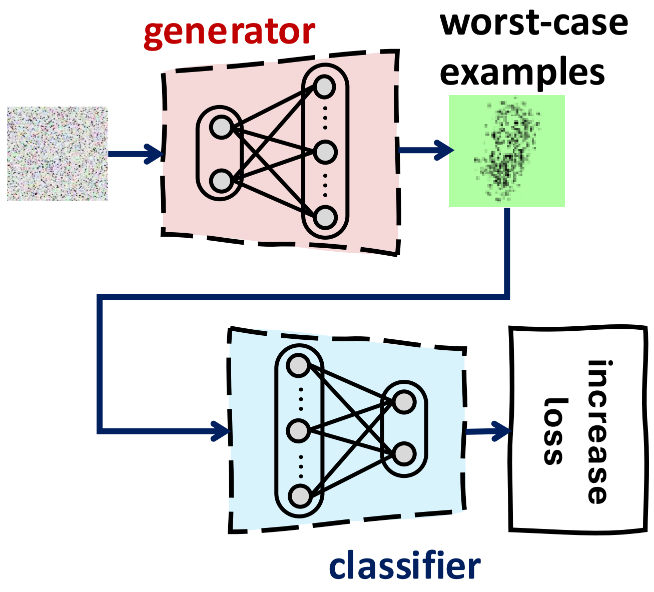

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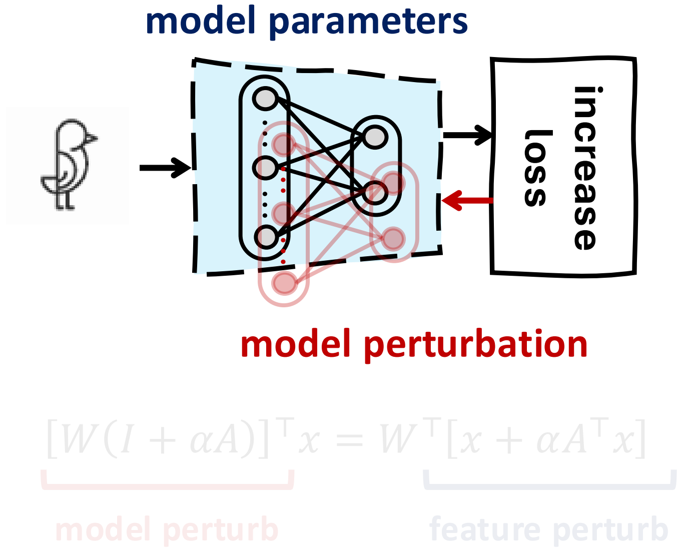

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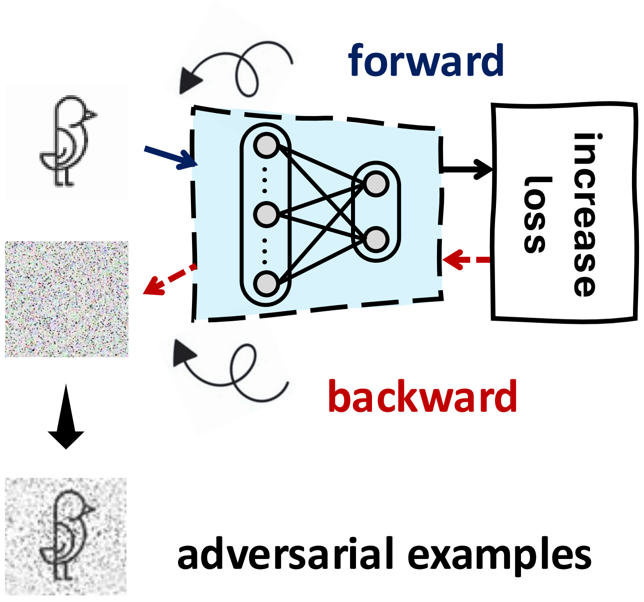

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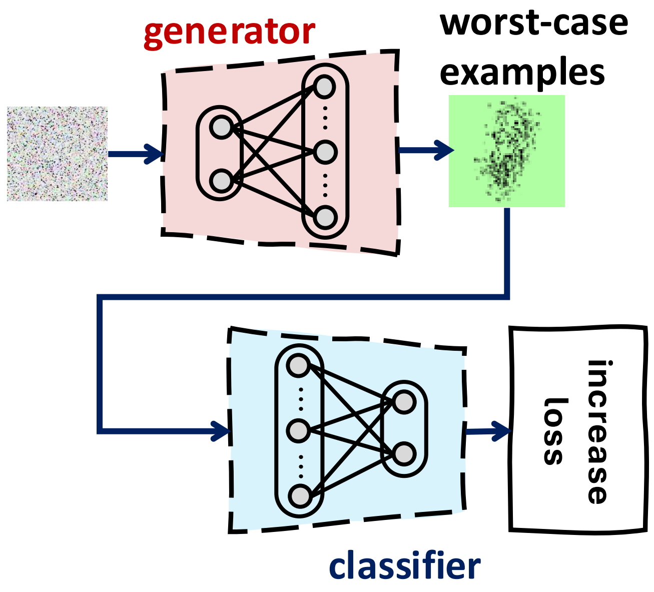
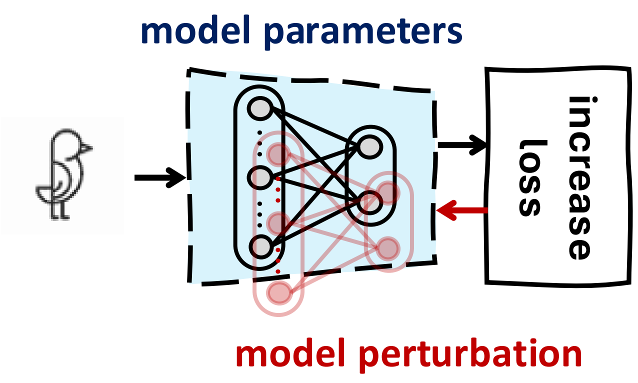


perturb latent embedding to maximize OOD loss values, thus creating worst-case examples.

❖ **Implicit Synthesis** [c]



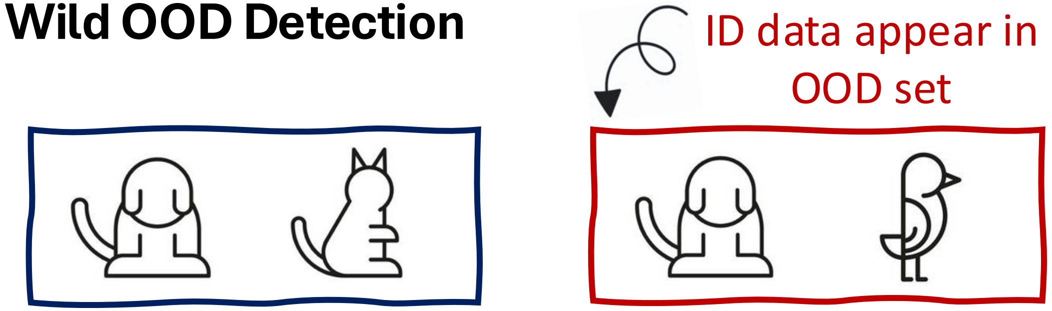
$$\underbrace{[W(I+\alpha A)]^\top}_{\text{model perturb}} x = W^\top \underbrace{[x+\alpha A^\top x]}_{\text{feature perturb}}$$

perturb parameters that maximize OOD loss can implicitly create worst-case examples.

[a] Zhu et al. Diversified Outlier Exposure for Out-of-distribution Detection via Informative Extrapolation. In NeurIPS, 2023.
[b] Lee et al. Training Confidence-calibrated Classifiers for Detecting Out-of-distribution Samples. In ICLR, 2018.
[c] Wang et al. Out-of-distribution Detection with Implicit Outlier Transformation. In ICLR, 2023.

Challenges and Future Directions

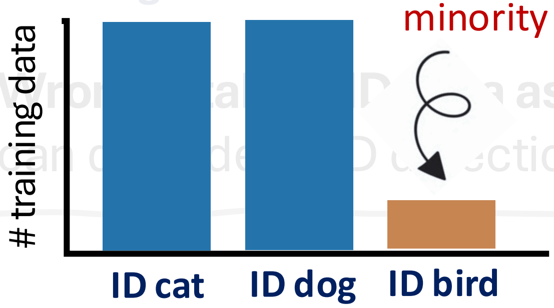
- **Wild OOD Detection**

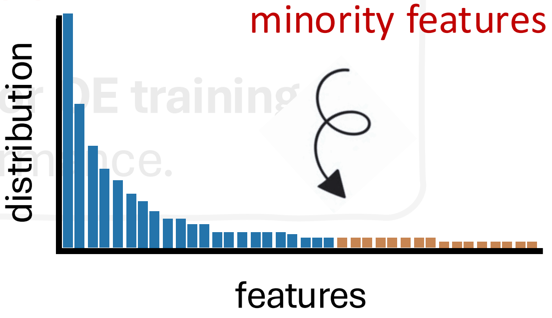


Wrongly taking ID data as OOD for OE training can degrade OOD detection performance.

Challenges and Future Directions

❖ **Imbalanced and Long-tailed OOD Learning**





Minority classes or features are easier to be confused with OOD data.

Challenges and Future Directions

❖ Wild OOD Detection

❖ Imbalanced and Long-tailed OOD Learning

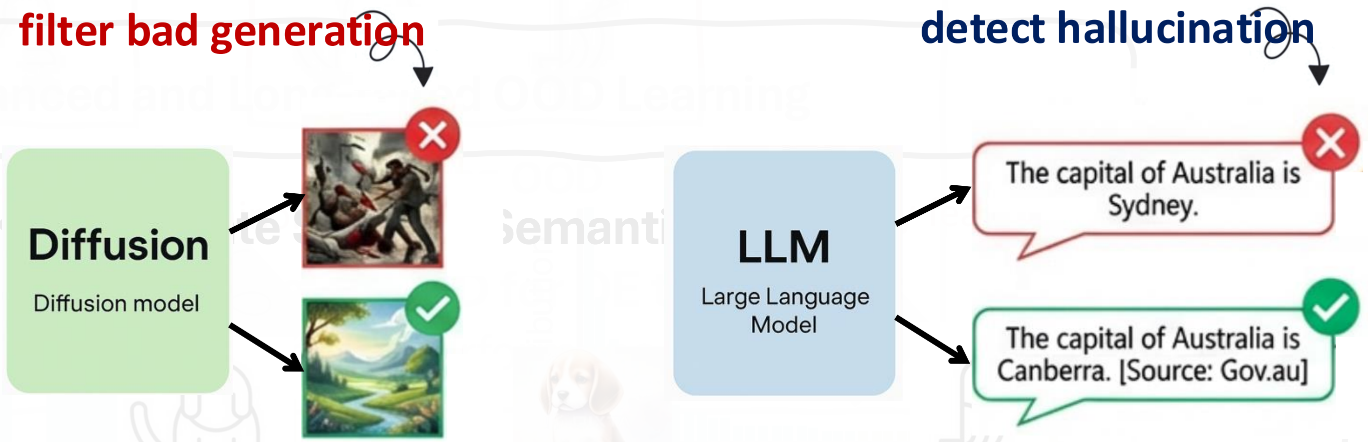
❖ **Covariate Shift vs. Semantic Shift**

ID covariate shift semantic shift (OOD)

Models typically **fail to discern data with covariate shift and semantic shift.**

Challenges and Future Directions

❖ **Large-scale Generative Models**



🤔 OOD detection can be used for **quality / safety control in large-scale generative models.**

Thank you for listening!

Find my slides from my homepage:
https://qizhouwang.github.io/homepage