OUT-OF-DISTRIBUTION DETECTION

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Problem Formulation

Out-of-distribution (OOD) detection in artificial neural networks addresses the critical challenge of ensuring model reliability when encountering inputs that deviate from the distribution on which the model was trained.

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Formal definition of the problem

Formally, consider a neural network model $f: \mathcal{X} \rightarrow \mathcal{Y}$ trained on a dataset $\mathcal{D}_{train} = \{(x_i, y_i)\}_{i=1}^{N}$ drawn from an in-distribution P_{in} .The goal of OOD detection is to distinguish between in-distribution samples $x \sim P_{in}$ and out-of-distribution samples $x \sim P_{ood}$,where $P_{ood} \neq P_{in}$.

The problem can be formulated as a binary classification task where the model must assign a confidence score $s(x)$ to each input x, such that:

- For in-distribution samples: $s(x)$ is high
- For out-of-distribution samples: $s(x)$ is low

OOD Challenges

- Neural networks tend to produce overconfident predictions even for OOD inputs
- The decision boundary between in- and out-of-distribution is not well-defined
- OOD detection must be performed without access to OOD data during training
- The method should be computationally efficient and applicable to various network architectures

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State-of-the-Art Methods

1. Maximum Softmax Probability (MSP)
2. ODIN (Out-of-Distribution Detector for Neural Networks)
3. Mahalanobis Distance-based Detection
4. Energy-based Out-of-Distribution Detection
5. Union of 1-Dimensional Subspaces (U1D)
6. Hyperdimensional Feature Fusion

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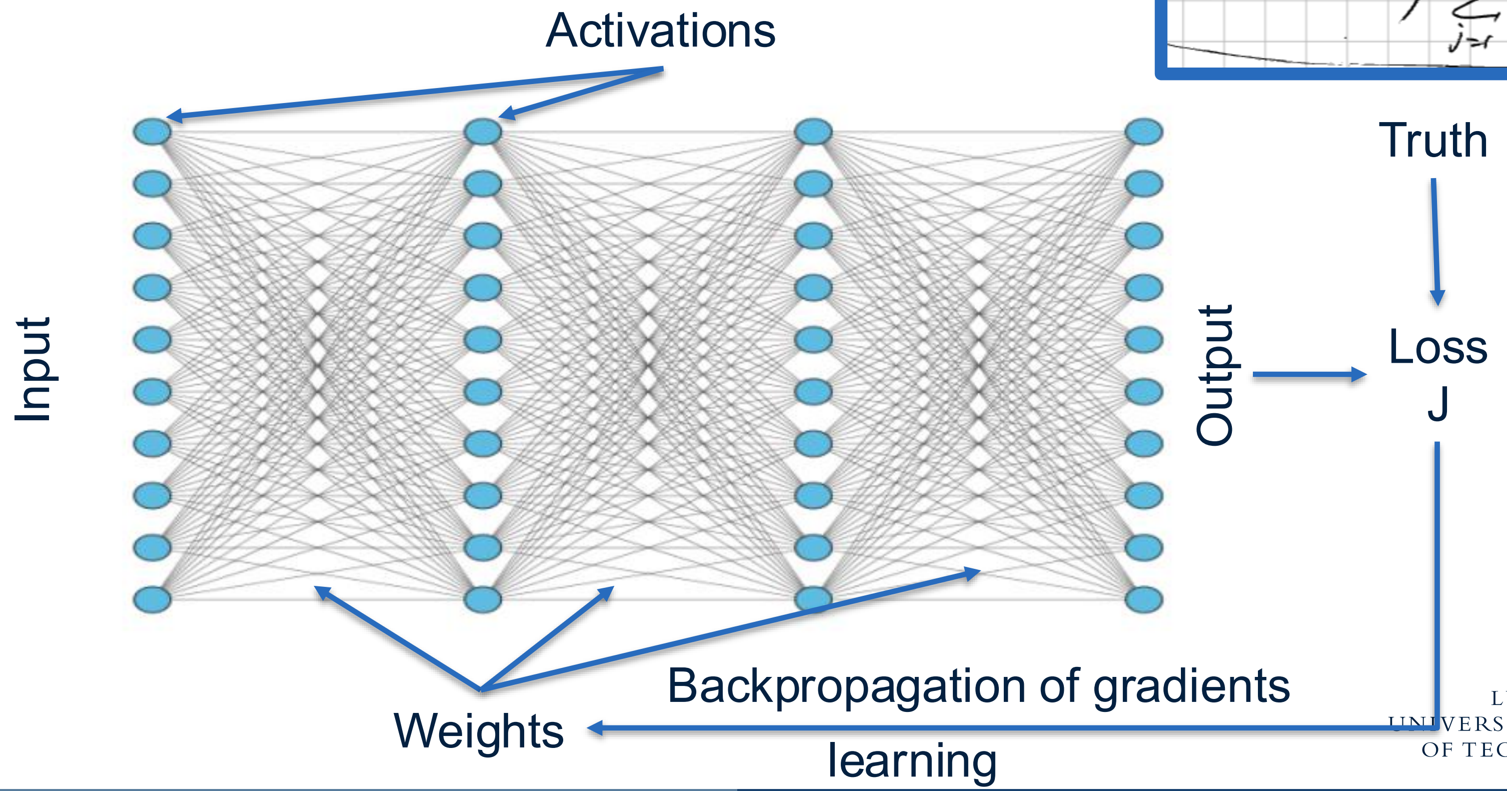
Maximum Softmax Probability (MSP)

Recall the output architecture in Artificial neural networks

SoftMax $S(x_i) = \frac{e^{x_i}}{\sum_{j=1}^{M} e^{x_j}}$



Maximum Softmax Probability (MSP)

Uses the maximum value of the softmax output as a confidence score. OOD samples typically have lower maximum probabilities due to the model’s uncertainty.

Example: For a 3-class classification, suppose an in-distribution sample has softmax outputs [0.05, 0.85, 0.10], yielding MSP = 0.85 (high confidence). An OOD sample might have [0.30, 0.35, 0.35], with MSP = 0.35 (lower confidence), indicating potential OOD.

ODIN (Out-of-Distribution Detector for Neural Networks)

ODIN improves upon MSP by applying **temperature** scaling to the softmax outputs and adding small perturbations to the input. This enhances the separation between in-distribution and OOD samples.

Effect of temperature:

$$S_i(x;T) = \frac{e^{f_i(x)/T}}{\sum_j e^{f_j(x)/T}}$$

When T≫1:

- Logits are scaled down
- Small logit differences matter more
- ID and OOD confidence gaps increase

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ODIN Example

Example: Using temperature T=1000, an in-distribution sample’s scaled softmax might be [0.001, 0.998, 0.001], while an OOD sample after perturbation could have [0.332, 0.334, 0.334]

A challenge

Traditional OOD methods:

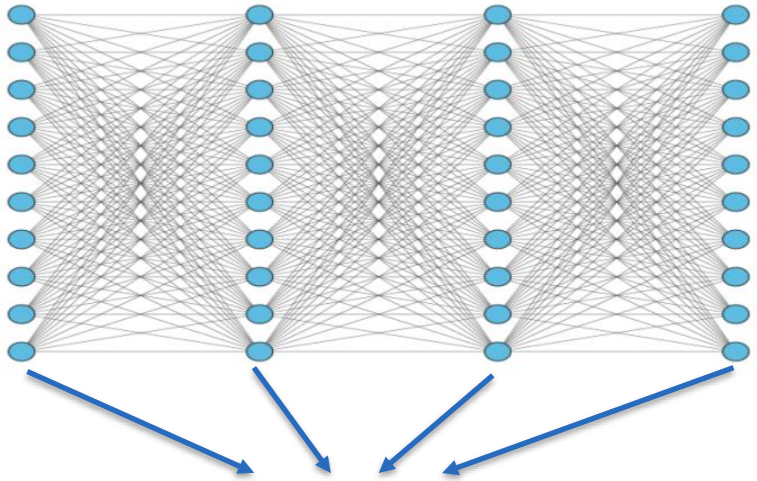
- MSP / ODIN operate on softmax outputs
- Mahalanobis operate on a single feature layer
- Energy-based operate on logits

Problem:

- Different layers encode **different types of information (for images)**
    - Early layers - low-level textures
    - Mid layers - shapes
    - Deep layers - semantics
- Single-layer OOD detection ignores this richness.

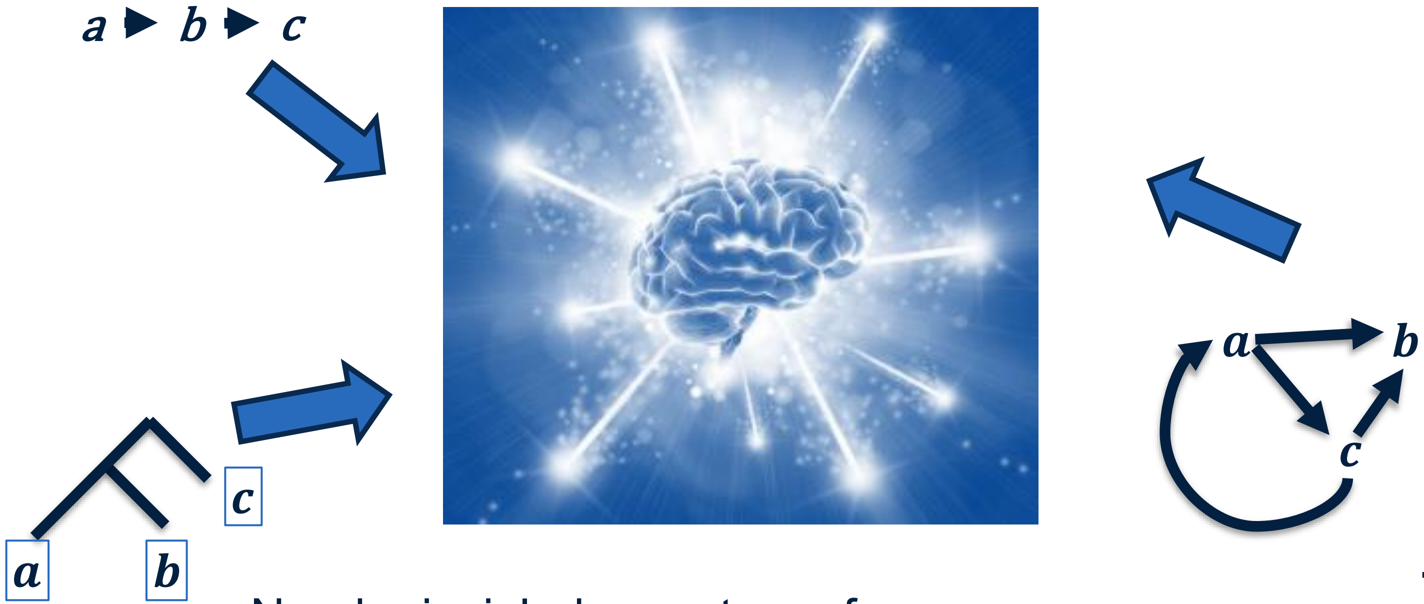
Hyperdimensional Feature Fusion

Idea: fuse features from multiple layers of the neural network into a single representation robust OOD detection.



Single vector representation

… based on methods of hyperdimensional computing



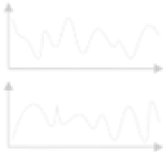
Need principled ways to perform computations on data structures in a brain-like manner

Principle 1: (Hyper)vectors

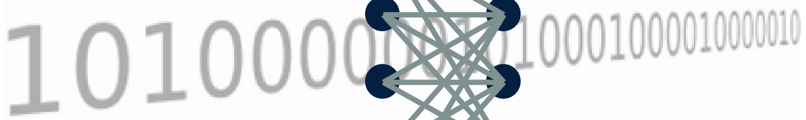
High-dimensional vectors appear everywhere in AI/ML pipelines

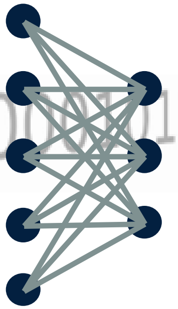
Data Representation → Model Representation → Similarity Measurement

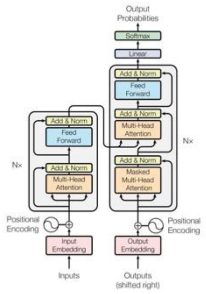
Images **Signals** **Text**

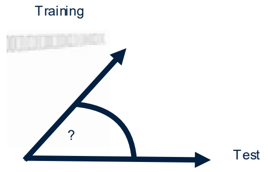


„Robot“









Hyperdimensional Computing (**HDC)** provides a **great toolbox** for handling them.

Hypervectors

- Let $\mathrm{a, b, c} \ldots \in \{\mathbb{B}^{\mathrm{D}}, \mathbb{R}^{\mathrm{D}}, \mathbb{C}^{\mathrm{D}}\}$,are vectors in D dimensional space
- D is high ($\sim 10^2, \sim 10^3, \sim 10^6, \ldots$)

- Operations:
- $a+b$:B$undling$ ($superposition$) (element-wise sum)
- $a \odot b$:B$inding$ (Hadamard product, XOR, Circular convolution)
- $a \oslash b$:U$nbinding\ operation$
- $\rho(a)$:O$rdering\ operation$ (permutation cyclic shift)

- similarity measure :Cosine similarity, Dot product, Hamming distance

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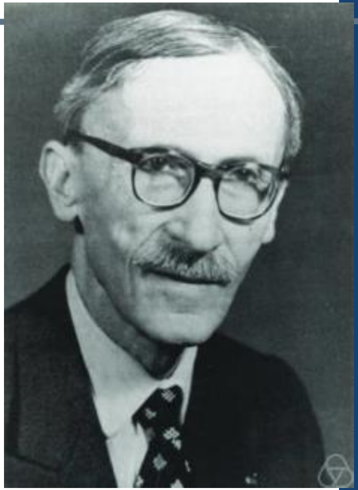
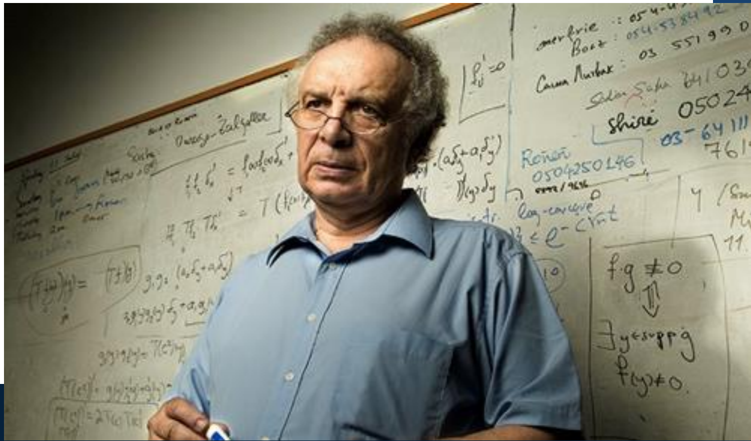
Principle 2: Concentration of Measure Theorems in VSA



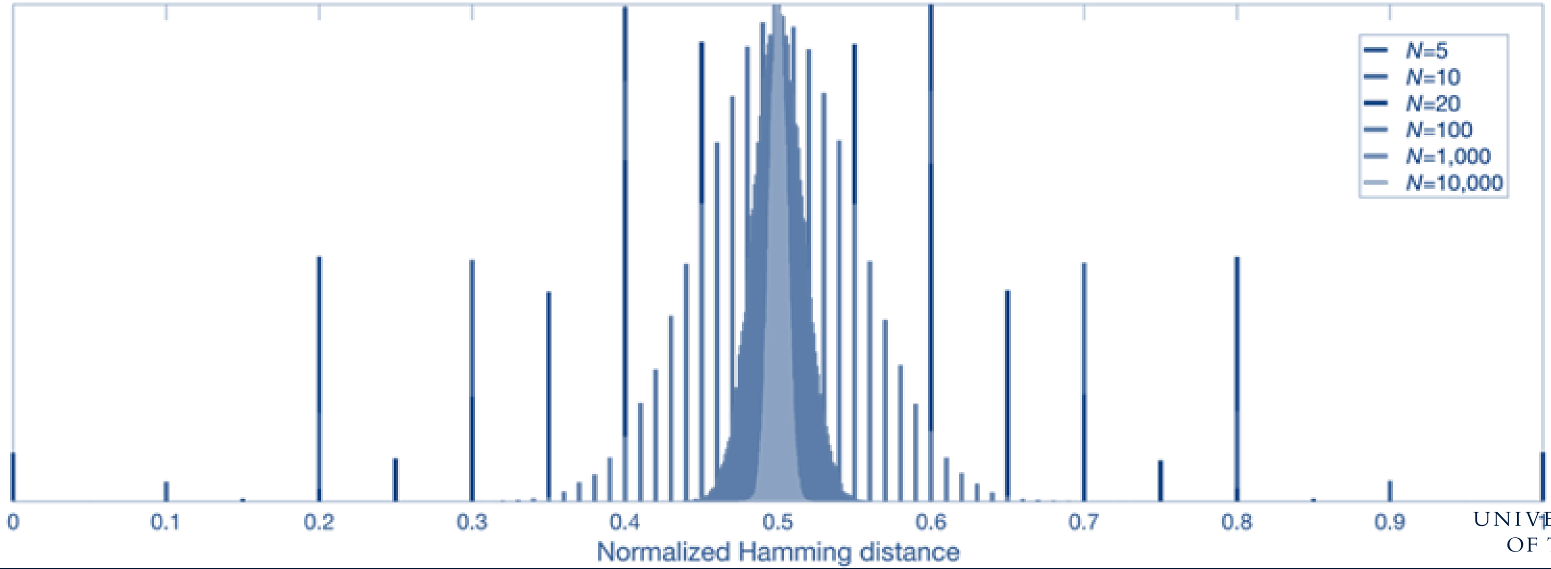
- Concentration of measure: In high dimensions, kernel of random vectors concentrate around their means
  - Paul Lévy
  - Vitali Milman

- Lévy's lemma: For unit vectors x, y on sphere,
  - $P(| < x, y > | \geq t) \leq 2\exp(-dt^2/2)$
- Implication: Random vectors are nearly orthogonal
- "Symbols" can be encoded as random vectors "for free"



Quasi-orthogonality is native in highdimensional random spaces – the case of B^N

- Higher is the dimensionality *N* the more stable is quasi-orthogonality between two random vectors
    - Gets thinner and thinner with increased *N*
    - Distribution of Hamming distance $\Delta_H(\mathbf{A},\mathbf{B})$ between randomly chosen HD vectors

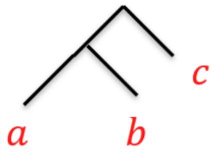


Principle 3: We can encode data structures with algebra on hypervectors

Sequence: $a \rightarrow b \rightarrow c$

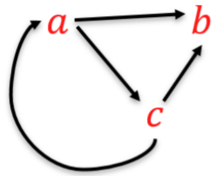
$$s = pos1 \odot a + pos2 \odot b + pos3 \odot c$$

Tree:



$$\boldsymbol{s} = \boldsymbol{r} \odot \boldsymbol{c} + \boldsymbol{l} \odot \boldsymbol{\rho}(\boldsymbol{l} \odot \boldsymbol{a}) + \boldsymbol{l} \odot \boldsymbol{\rho}(\boldsymbol{r} \odot \boldsymbol{b})$$

Graph:



$$\boldsymbol{s} = \boldsymbol{a} \odot \boldsymbol{\rho}(\boldsymbol{b}) + \boldsymbol{a} \odot \boldsymbol{\rho}(\boldsymbol{c}) + \boldsymbol{c} \odot \boldsymbol{\rho}(\boldsymbol{b}) + \boldsymbol{c} \odot \boldsymbol{\rho}(\boldsymbol{a})$$

Similarity between hypervectors captures similarity between data structures

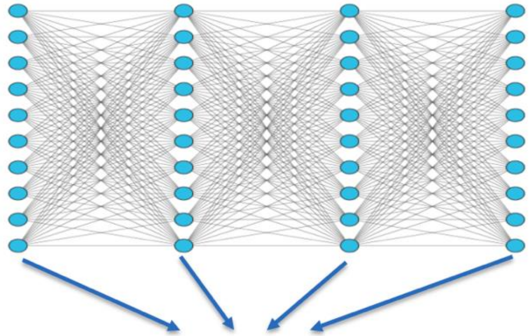
Layer Encoding via Binding

Each layer gets a unique random hypervector key: k_l

Then bind:

$$z_l = k_l \odot h_l$$

($\odot$ = element-wise multiplication)



Single vector representation

- This preserves layer identity.
- Dimensionality of layer representations h_l should be aligned – random projection

Bundling (Superposition)

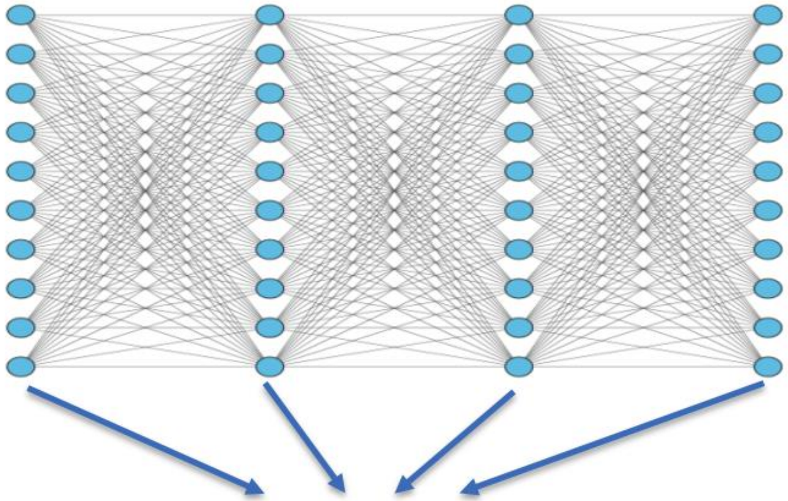
Final input descriptor:

$$y = \sum_{l=1}^{L} z_l$$

Optionally apply sign function:

y=sign(y)

- In this way y is a single vector representing a list of layers L



Single vector representation

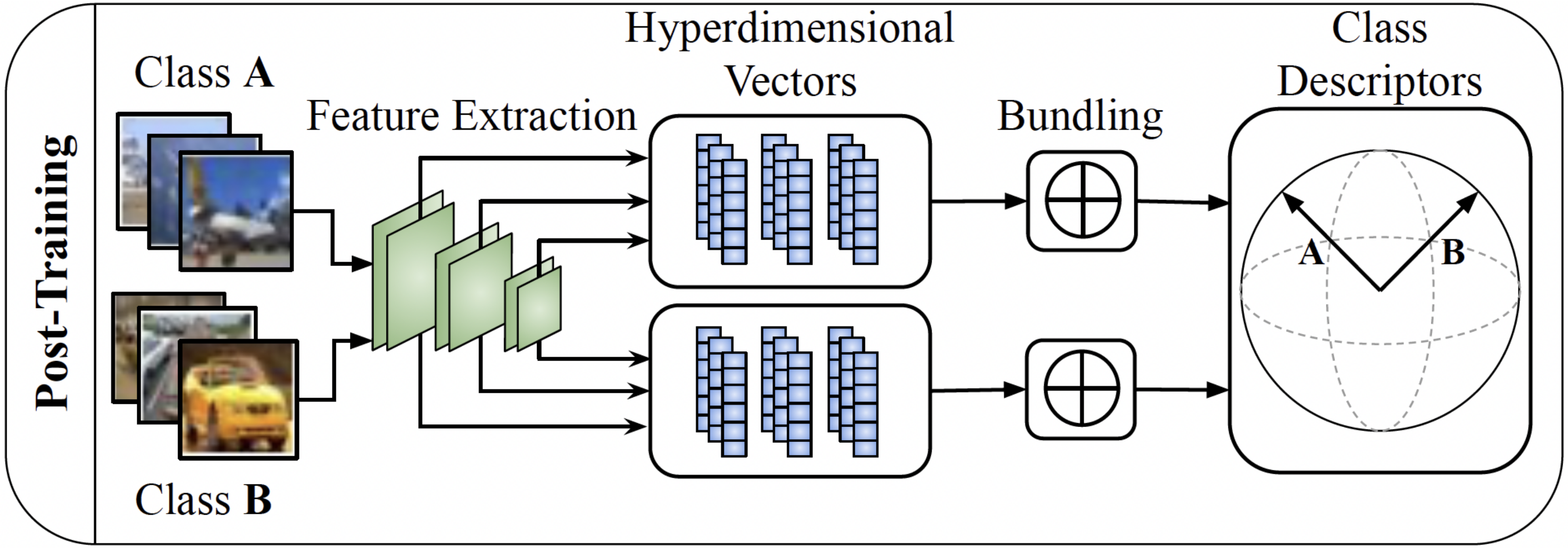
OOD scoring

For test sample:

1. Compute fused hypervector y
2. Compute similarity to prototypes: $s_c = \cos(y, \mu_c)$
3. Define OOD score: $\mathrm{Score}(\mathrm{x}) = \max_c s_c$

- Low similarity means OOD.

Post-training phase



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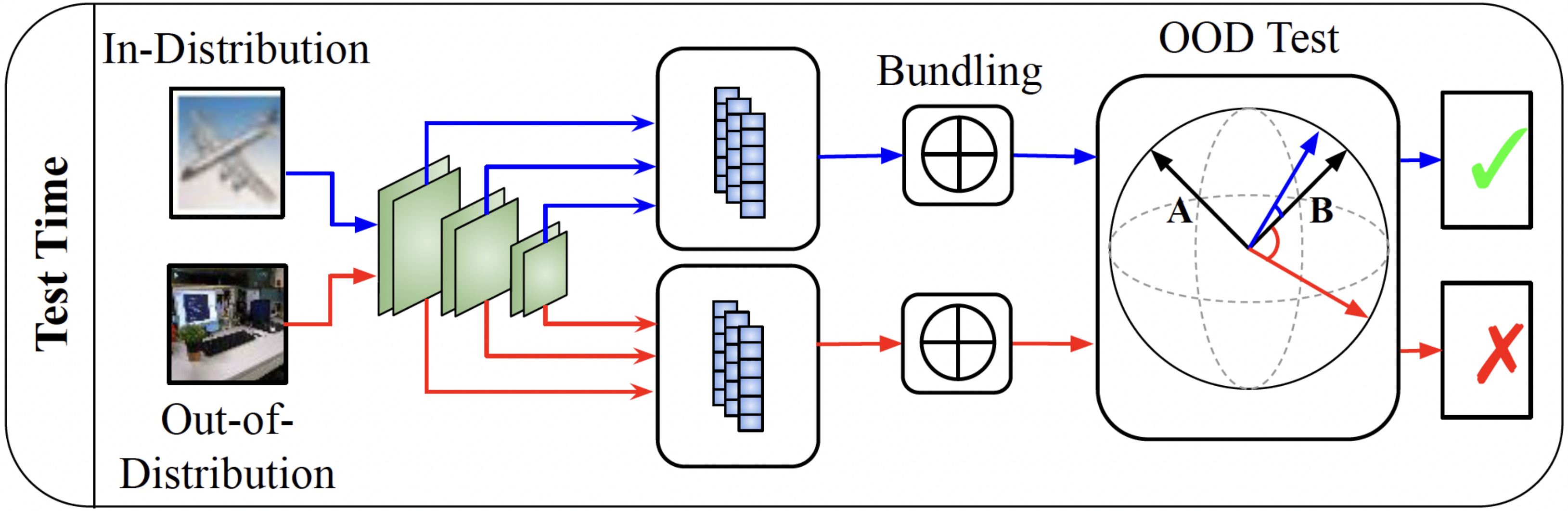
Test time



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References

- Wilson et al. (2022). Hyperdimensional Feature Fusion for Out-of-Distribution Detection. arXiv:2112.05341.