

ESCAPING LOW-RANK TRAPS: INTERPRETABLE VISUAL CONCEPT LEARNING VIA IMPLICIT VECTOR QUANTIZATION

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ABSTRACT

Concept Bottleneck Models (CBMs) achieve interpretability by interposing a human-understandable concept layer between perception and label prediction. The foundation of CBMs lies in the many-to-many mapping that translates high-dimensional visual features to a set of discrete concepts. However, we identify a critical and pervasive challenge that undermines this process: *representational collapse*, where visual patch features degenerate into a low-rank subspace during training, severely degrading the quality of learned concept activation vectors, thus hindering both model interpretability and downstream performance. To address these issues, we propose Implicit Vector Quantization (IVQ), a lightweight regularizer that maintains high-rank, diverse representations throughout training. Rather than imposing a hard bottleneck via direct quantization, IVQ learns a code-book prior that anchors semantic information in visual features, allowing it to act as a proxy objective. To further exploit these high-rank concept-aware features, we propose Magnet Attention, which dynamically aggregates patch-level features into visual concept prototypes, explicitly modeling the many-to-many vision-concept correspondence. Extensive experimental results show that our approach effectively prevents representational collapse and achieves state-of-the-art performance on eight diverse benchmarks. Our experiments further probe the low-rank phenomenon in representational collapse, finding that IVQ mitigates the information bottleneck and yields cross-modal representations with clearer, more interpretable consistency.

1 INTRODUCTION

Explainable Artificial Intelligence (xAI) aims to embed neural networks with *human-interpretable* and *interactive* reasoning processes, thereby opening the *black box* of end-to-end prediction systems. Among the ante-hoc xAI methods, the **Concept Bottleneck Model** (CBM) (Koh et al., 2020) is a prominent approach that pipelines predictions through an intermediate *concept layer*. This layer, situated between a perceptual encoder and a final task head, forces the model to operate in two distinct stages: First, a *perception* stage maps inputs to a set of predefined semantic concepts (e.g., *shape of a beak* or *spatial extent of a lesion*). Second, a *reasoning* stage uses only these concept activation vectors (CAVs) to make the final decision.

In the two-stage learning, perception and modeling of CAVs in the initial stage is foundational. The core of this stage lies in constructing a cross-modal patch-concept alignment process, which compels the model to learn the mapping and disentanglement of raw, high-dimensional visual embeddings into a set of structured visual representation vectors corresponding to human-defined concepts. As illustrated in [Figure 1a](#), an intrinsic many-to-many correspondence exists between local visual features and high level semantic concepts within the cross-modal concept alignment. The relationship is two-fold: an individual image patch may map to multiple concepts, while concurrently, the visual representation of a single concept is distributed across several distinct image patches. However, previous methods such as ([Yang et al., 2023](#); [Yuksekgonul et al., 2023](#); [Oikarinen et al., 2023](#); [Sheth & Kahou, 2023](#)) employ a visual encoder to extract a single global embedding for concept alignment. Due to the limited expressiveness of a single visual feature, these approaches fail to explicitly model the complex many-to-many mapping between local features and high-level concepts.

However, when we attempt to explicitly construct this relationship, a critical phenomenon termed *representational collapse* emerges, severely impeding the process. As presented in Figure 1b, we tracked the rank of the patch feature matrix throughout the training; the rank undergoes a sharp decline during the initial epochs on both training and validation sets, eventually bottoming out at a rank of 70, a drastic reduction from the potential full rank of 196. This behavior is not an anomaly; as shown in Figure 1c, concurrent works such as ExplicD (Gao et al., 2024) and MVP-CBM (Wang et al., 2025) exhibit a similar pattern, suggesting that *representational collapse* is a fundamental obstacle in this domain. Meanwhile, its essence is a symptom of a more fundamental problem: the collapse of feature diversity. This collapse is particularly damaging for CBMs, as a degenerated representation space lacks the expressive capacity to encode a diverse set of concepts (Sansone et al., 2025). When visual feature embeddings become highly similar and informationally redundant, the learning process itself is confounded (Jing et al., 2022), directly inhibiting the formation of high-quality, disentangled visual features, which are the foundation of the CBM.

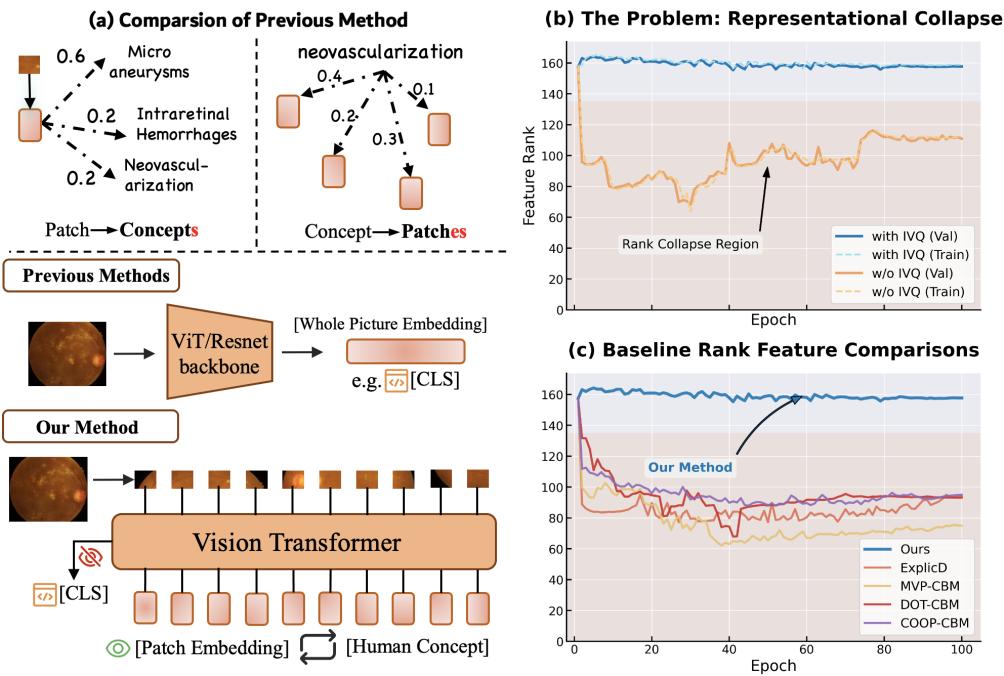


Figure 1: (a) An illustration of many-to-many cross-modal alignment in CBMs. (b) Comparison of feature rank dynamics during training on the training and validation sets, with and without IVQ. (c) Feature rank dynamic comparisons with previous baselines.

Hence, we introduce Implicit Vector Quantization (IVQ), a novel regularizer that repurposes the VQ objective as a loss term without quantizing the forward pass. The loss effectively forms a semantic bridge, compelling each patch feature to align with the nearest learned codebook prototype. Collectively, these prototypes act as distinct anchors that prevent the feature distribution from collapsing into a degenerate subspace. As depicted in Figure 1b and c, this directly counters representation collapse by maintaining a stable and elevated feature rank throughout training. Furthermore, building upon concept-aware, well-structured visual features, we introduce a Magnet Attention mechanism, which dynamically aggregates the diverse patch-level features into a holistic, semantically coherent visual representation prototype for each pre-defined textual concept, effectively modeling the many-to-many mapping.

This work makes three key contributions:

- We identify that the key to CBMs lies in modeling the many-to-many relationship between concepts and patches. Furthermore, we identify and analyze *representational collapse*, a key challenge in training modern CBMs that hinders the establishment of CAVs.
- We propose IVQ, a novel regularization method that preserves feature diversity and prevents representational collapse without creating an information bottleneck. To exploit ob-

108 tained rich representations, we introduce the Magnet Attention mechanism to effectively
 109 aggregate the regularized patch features into semantically meaningful concept prototypes.
 110

- 111 • Extensive experiments on **eight benchmarks** demonstrate that our IVQ-CBM consistently
 112 outperforms **eight strong baselines**, achieving state-of-the-art accuracy and learning better
 113 interpretable representations consistent with textual concepts.

114 2 RELATED WORK

115 **Concept Bottleneck Model.** It achieves interpretability-by-design by introducing a human-defined
 116 concept layer that bridges raw visual features and human-understandable semantics, providing a
 117 foundational explanation for the model’s final decision (Koh et al., 2020). A key challenge lies in
 118 achieving high-quality cross-modal alignment, *i.e.*, constructing a precise, fine-grained mapping be-
 119 tween visual features and textual concepts. However, many popular methods (Yuksekgonul et al.,
 120 2023; Oikarinen et al., 2023) rely on a single, holistic visual feature, such as the [CLS] token from
 121 CLIP-style models or a global image embedding from visual foundation models (Kim et al., 2023).
 122 These approaches operate on the premise that a global feature vector encapsulates all necessary
 123 visual attributes (Zhang et al., 2014; Raghu et al., 2022). This assumption is untenable in com-
 124 plex visual scenes, especially for medical images characterized by subtle, intricate, and fragmented
 125 lesions (Chen et al., 2021).

126 To establish a more fine-grained, many-to-many mapping, recent works have begun to leverage
 127 patch-level embeddings from Vision Transformers (ViTs) (Dosovitskiy et al., 2021), which offer a
 128 powerful prior for perception and alignment. Several works have ventured in this direction, em-
 129 ploying techniques such as Optimal Transport (Xie et al., 2025), or Cross-Attention and dynamic
 130 pooling to learn visual concepts (Wang et al., 2025; Gao et al., 2024), yet a critical issue arises: the
 131 visual features extracted from the encoder suffer from **representational collapse**, a phenomenon
 132 where the feature vectors degenerate into a low-dimensional subspace, becoming informationally
 133 redundant and lacking diversity.

134 **Representation Regularization.** Low-rank issue has been extensively studied in the self-supervised
 135 learning (SSL) literature. For instance, Barlow Twins (Zbontar et al., 2021) mitigates collapse by
 136 minimizing the redundancy between feature dimensions via a cross-correlation matrix. Other tech-
 137 niques, such as spectral regularization (Yoshida & Miyato, 2017), constrain the spectral norm of
 138 weight matrices to improve generalization. A more recent work DINOv3 (Siméoni et al., 2025) in-
 139 troduces gram regularization loss to prevent the model’s output from collapsing to a trivial solution.

140 Nevertheless, a critical drawback exists in directly applying these techniques to CBMs: they are not
 141 tailored for the specific demands of the CBM task, nor are they designed for cross-modal, many-
 142 to-many alignment. Specifically, the core objective of these regularization methods is to *indiscrimi-*
 143 *nately* maximize feature diversity or reduce redundancy (Huang et al., 2017; Gao & Pu, 2025). For
 144 CBMs, however, the goal is not arbitrary diversity, but rather **meaningful, structured diversity** that
 145 aligns with human-defined concepts. Indiscriminate decorrelation or spectral regularization cannot
 146 guarantee that the learned feature diversity has any correspondence with the predefined semantic
 147 concepts. Consequently, these methods may amplify trivial visual details that are useless or even
 148 detrimental to the final task, thereby interfering with the formation of high-quality concept vectors
 149 (as we demonstrate in Section 4.2).

150 **Vector Quantization.** VQ has played a central role in learning discrete latent representations.
 151 Early work on Neural Discrete Representation Learning (Van Den Oord et al., 2017a) introduced
 152 codebook-based quantization that enables end-to-end training through a nearest-neighbor commit-
 153 ment objective. Follow-up variants such as VQ-VAE-2 (Razavi et al., 2019) further enhanced gener-
 154 ative fidelity via multi-level discrete hierarchies. Beyond architectural extensions, a series of studies
 155 examined the optimization challenges of VQ. Rotation-based VQ (Fifty et al., 2025) restructures
 156 the quantization space to stabilize code assignments, whereas linear-layer VQ (Zhu et al., 2025)
 157 proposes lightweight transformations to mitigate representation collapse and improve codebook
 158 utilization. VQ has also been explored within broader perceptual tasks: Vector-Quantized Vision
 159 Foundation Models (Zhao et al., 2025) leveraged discrete visual tokens for object-centric learning,
 160 and scaling studies, such as 100k-VQGAN (Zhu et al., 2024), demonstrated that extremely large
 161 codebooks can maintain high utilization. More recent designs like MGVQ (Jia et al., 2025) adopt
 162 multi-group quantization to increase representational granularity and improve generalization.

Despite these advances, prior works rely on explicit quantization, where the quantized vectors replace continuous features in the forward pass. Such a hard discrete bottleneck is often beneficial for generative modeling but is misaligned with CBMs, which require preserving rich, distributed semantic information and allowing many-to-many relations between patches and concepts.

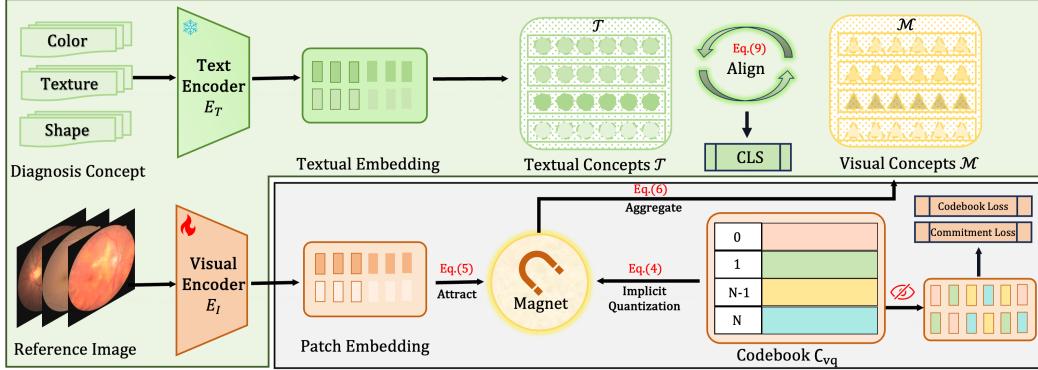


Figure 2: A pipeline of the proposed IVQ-CBM method which optimizes training from three dimensions: classification accuracy, concept alignment, as well as representation diversity and quality. An many-to-many mapping between visual embeddings and textual concepts establish the foundation of our model. IVQ further regularizes the representation space and helps to maintain and distill the core information for each patch throughout training. Building upon obtained high-rank concept-aware features, magnet aggregates visual concepts from raw embeddings, regarded as input for concept alignment and final classification.

3 METHODOLOGY

3.1 PRELIMINARIES AND OVERALL FRAMEWORK

Problem Formulation. Consider a dataset of triplets $\mathcal{D} = \{(x_i, c_i, y_i)\}_{i=1}^N$, where $x_i \in \mathcal{X}$ is an input image, $y_i \in \mathcal{Y}$ denotes the corresponding class label, and c_i is a set of textual descriptions defining the concepts associated with class y_i . In contrast to standard black-box models that directly learn a mapping $x_i \rightarrow y_i$, the CBM pipeline is formulated as a two-stage process: $x_i \rightarrow c_i \rightarrow y_i$. First, the alignment stage produces a CAV, which we denote as $\mathbf{v}_i \in \mathbb{R}^K$. This vector contains the activation scores for all K concepts for a given image x_i . It is generated by aligning the learned Visual Concepts, $\mathcal{M} \in \mathbb{R}^{K \times D}$, with their corresponding textual concept embeddings, $\tau \in \mathbb{R}^{K \times D}$. Specifically, the activation score for the k -th concept is computed as the dot product between its visual and textual representations:

$$(\mathbf{v}_i)_k = \mathcal{M}_k \cdot \tau_k, \quad \forall k \in \{1, \dots, K\}. \quad (1)$$

The CAVs then serve as the exclusive input for the second-stage classification task. Given the straightforward mechanism of the second stage, achieving precise and efficient image-concept alignment in the first stage is of paramount importance.

Visual Concept Learning. To acquire fine-grained visual features, we leverage a pre-trained CLIP ViT encoder to obtain a structured visual representation from the input image x_i :

$$\mathbf{Z}_v = [\mathbf{z}_{\text{cls}}, \mathbf{z}_1, \mathbf{z}_2, \dots, \mathbf{z}_L] = E_I(x_i) \in \mathbb{R}^{(L+1) \times D}. \quad (2)$$

where \mathbf{z}_{cls} is the class token embedding and $\mathbf{Z}_p = [\mathbf{z}_1, \dots, \mathbf{z}_L] \in \mathbb{R}^{L \times D}$ represents the matrix of patch token embeddings. This patch-level representation is crucial, as a single textual concept often corresponds to information spanning multiple patches, while a single patch may contain details relevant to multiple concepts.

This complex, many-to-many mapping necessitates a sophisticated mechanism to bridge the gap between local features and high-level concepts. Therefore, our objective is to aggregate the patch features \mathbf{Z}_p into K meaningful **Visual Concepts**, denoted by the matrix $\mathcal{M} \in \mathbb{R}^{K \times D}$. These learned Visual Concepts are subsequently used for the final concept-text alignment as described in our problem formulation. The following sections detail the two core components of our method designed to achieve this: IVQ for representation regularization and the Magnet Attention mechanism for concept aggregation.

216 3.2 IMPLICIT VECTOR QUANTIZATION
217

218 To mitigate the aforementioned issues, we propose a novel IVQ mechanism. In contrast to conventional
219 VQ approaches, which first identify the nearest codebook vector over a distance metric and
220 subsequently propagate the resulting quantized features through the forward pass, our IVQ method
221 strategically discards the quantized features. Instead, it exclusively leverages the commitment and
222 codebook losses as regularization terms during backpropagation. This process compels each visual
223 patch embedding to align more closely with its nearest codebook vector—which semantically cor-
224 responds to a textual concept, as will be verified in our [Section 4.2](#). This, in turn, distills the core
225 conceptual information while simultaneously regularizing the representation space and enhancing
226 the diversity of visual features, ultimately benefiting the subsequent aggregation of visual concepts.
227

228 Given the encoded visual patch features $\mathbf{Z}_p = \{\mathbf{z}_j\}_{j=1}^L$, a critical challenge is to prevent representa-
229 tion collapse and enhance feature diversity. We maintain a small, learnable codebook $\mathcal{C}_{vq} \in \mathbb{R}^{M \times D}$,
230 where M equals the number of textual concepts K (discussed in [Section 4.2](#)). For each patch feature
231 $\mathbf{z}_j \in \mathbf{Z}_p$, we find the nearest codebook vector $\mathbf{c}_k \in \mathcal{C}_{vq}$ via an $\arg\min$ operation over the Euclidean
232 distance:

$$k_j = \arg\min_k \|\mathbf{z}_j - \mathbf{c}_k\|_2^2. \quad (3)$$

233 The quantized representation $\mathbf{z}_{q,j} = \mathbf{c}_{k_j}$. However, we discard this quantized output \mathbf{Z}_q and do
234 not use it in the subsequent forward pass. Instead, we compute the VQ loss, which consists of a
235 codebook loss and a commitment loss, to update the feature encoder and \mathcal{C}_{vq} :

$$\mathcal{L}_{IVQ} = \underbrace{\|\text{sg}(\mathbf{Z}_p) - \mathbf{Z}_q\|_2^2}_{\text{Codebook Loss}} + \beta \underbrace{\|\mathbf{Z}_p - \text{sg}(\mathbf{Z}_q)\|_2^2}_{\text{Commitment Loss}}, \quad (4)$$

236 where $\text{sg}(\cdot)$ denotes the stop-gradient operator and β is the commitment cost hyperparameter. By
237 backpropagating \mathcal{L}_{IVQ} , we compel the patch features in \mathbf{Z}_v to align with a learned prototype without
238 suffering from the information bottleneck of hard quantization. This process regularizes the repre-
239 sentation space, encouraging a more structured and diverse feature distribution, which is crucial for
240 the subsequent aggregation stage.

241 3.3 MAGNET CONCEPT AGGREGATION
242

243 With a regularized, high-rank feature space established by IVQ, we now introduce a mechanism
244 to bridge the gap between low-level visual features and high-level semantic concepts. A simple
245 spatial pooling of all patch features would lose critical fine-grained information ([Wang et al., 2025](#)).
246 Therefore, we propose the **Magnet Attention** mechanism, a differentiable soft-clustering module
247 designed to aggregate the L patch features into K semantically meaningful Visual Concepts.
248

249 To achieve this, we first introduce a set of learnable **concept queries**, denoted as $\mathbf{Q} \in \mathbb{R}^{K \times D}$, where
250 K is the number of concepts. Each query vector $\mathbf{q}_k \in \mathbf{Q}$ acts as a learnable center-point to attract
251 patch features related to a specific concept. For the input patch features $\mathbf{Z}_p = \{\mathbf{z}_j\}_{j=1}^L$, we compute
252 a similarity score between each patch feature \mathbf{z}_j and each concept query \mathbf{q}_k . Following common
253 practice, we use negative squared Euclidean distance as the similarity metric ([Van Den Oord et al., 2017b](#)).
254

255 This similarity is then converted into a soft assignment matrix $\mathbf{A} \in \mathbb{R}^{L \times K}$ via a softmax function
256 over the concepts:

$$A_{jk} = \frac{\exp(-\|\mathbf{z}_j - \mathbf{q}_k\|_2^2)}{\sum_{k'=1}^K \exp(-\|\mathbf{z}_j - \mathbf{q}_{k'}\|_2^2)}, \quad (5)$$

257 where A_{jk} represents the soft-assignment weight of the j -th patch to the k -th concept query. These
258 weights form an attention map over the patches for each concept. The final **Visual Concepts**, de-
259 noted by the matrix $\mathcal{M} \in \mathbb{R}^{K \times D}$, are then computed as a weighted average of the patch features:

$$\mathcal{M} = \mathbf{A}^\top \mathbf{Z}_p. \quad (6)$$

260 The resulting matrix \mathcal{M} contains K rich visual concept prototypes, each summarizing the relevant
261 spatial information from the image corresponding to a distinct semantic concept. This aggregated
262 representation \mathcal{M} is then used for the final alignment with the textual concept embeddings τ .

270 3.4 TRAINING OBJECTIVES
271272 We train our model end-to-end with a composite loss that simultaneously optimizes for task accu-
273 racy, concept alignment, and representation quality.
274275 **Classification Loss.** The primary objective is to ensure the model accurately performs the final
276 classification task. Let h_{cls} denote the final classification head. It takes the vector of concept activa-
277 tion scores $\mathbf{v}_i \in \mathbb{R}^K$ as input to produce the final class logits $\mathbf{p}_i = h_{\text{cls}}(\mathbf{v}_i)$. As defined previously,
278 each score $(\mathbf{v}_i)_k$ represents the alignment between the k -th visual concept and the k -th textual con-
279 cept. The classification loss \mathcal{L}_{cls} is the standard cross-entropy between the predicted logits and the
280 ground-truth class label y_i :

281
$$\mathcal{L}_{\text{cls}} = \mathcal{L}_{\text{CE}}(\mathbf{p}_i, y_i). \quad (7)$$

282 **Concept Alignment Loss.** To ensure the model’s interpretability, we explicitly supervise the con-
283 cept bottleneck. The concept activation scores $\mathbf{v}_i \in \mathbb{R}^K$ serve as the logits for concept prediction.
284 We supervise these logits against the ground-truth concept labels $\mathbf{c}_i \in \{0, 1\}^K$, which is a multi-hot
285 vector indicating the presence of each of the K concepts for the sample x_i . The concept alignment
286 loss $\mathcal{L}_{\text{concept}}$ is the binary cross-entropy (BCE) loss between the predicted concept scores and the
287 ground-truth labels:

288
$$\mathcal{L}_{\text{concept}} = \mathcal{L}_{\text{BCE}}(\mathbf{v}_i, \mathbf{c}_i). \quad (8)$$

289 This loss is crucial as it forces the model to learn a set of visually grounded and semantically mean-
290 ingful concepts.
291292 **IVQ Regularization Loss.** As detailed previously, the \mathcal{L}_{IVQ} encourages the patch-level features
293 to form a more structured and diverse representation space without introducing a hard information
294 bottleneck. This improves the robustness of the feature extractor and aids the Magnet Attention
295 mechanism in forming higher-quality Visual Concepts.
296297 **Overall Training Objective.** The final training objective combines these three components into a
298 single multi-task loss function. The total loss \mathcal{L} is formulated as a weighted sum:
299

300
$$\mathcal{L} = \mathcal{L}_{\text{cls}} + \mathcal{L}_{\text{concept}} + \mathcal{L}_{\text{IVQ}}. \quad (9)$$

301 4 EXPERIMENTS AND DISCUSSIONS
302303 **Core Questions.** We structure our analysis around a series of research questions (RQs) to thoroughly
304 investigate the properties and efficacy of our proposed method. Our goal is to dissect its underlying
305 mechanisms, justify its design choices, and demonstrate its advantages in terms of performance and
306 interpretability.
307308 **RQ1: Impact on Representation Collapse.** How does implicit quantization affect the rank of the
309 learned representations? [Figure 4](#) and [6](#).310 **RQ2: Efficacy of Implicit Quantization.** Is implicit quantization a genuinely effective technique?
311 How does it conceptually and empirically differ from explicit quantization? [Section 4.2](#)312 **RQ3: Implicit Quantization as a Regularizer.** Our method can be interpreted as a form of repre-
313 sentation space regularization. How does its performance compare against other established
314 regularization techniques? Why does our proposed implicit quantization, which leverages a
315 codebook, outperform traditional regularization techniques on CBM? [Section 4.2](#)316 **RQ4: Optimal Codebook Configuration.** The core component of our method is the codebook, which
317 is dynamically updated throughout training. What is the optimal relationship between the code-
318 book size, M , and the number of textual concept vectors, K ? [Section 4.2](#)319 **RQ5: Interpretability as a Visual Dictionary.** Beyond performance, how does the codebook con-
320 tribute to model interpretability? [Section 4.2](#)
321322 **Baselines, Benchmarks, and Metrics.** To comprehensively evaluate the robustness and general-
323 ization of our method, we conduct experiments on a diverse suite of public benchmarks spanning
two distinct domains. First, for **medical imaging**, we utilize datasets covering dermoscopy ([Codella](#)

et al., 2019), histopathology (Kather et al., 2018), fundus photography (Porwal et al., 2018; yiweichen04, 2021), ultrasound (Al-Dhabayani et al., 2020), chest X-ray (Zawacki et al., 2019; Johnson et al., 2019), and mammography (Cui et al., 2021). Second, to demonstrate the broad **generalizability** of IVQ-CBM to natural images, we extend our evaluation to five standard computer vision benchmarks: CIFAR-10 and CIFAR-100 (Krizhevsky, 2009) for general object classification, CUB-200-2011 (Wah et al., 2011) for fine-grained identification, Places365 (Zhou et al., 2017) for scene recognition, and ImageNet-1K (Russakovsky et al., 2015) for large-scale classification.

To demonstrate its effectiveness, we benchmark our approach against eight recent and popular CBM methods: LaBo (Yang et al., 2023), PCBM (Yuksekgonul et al., 2023), COOP-CBM (Sheth & Kaghani, 2023), LF-CBM (Oikarinen et al., 2023), Explid (Gao et al., 2024), MVP-CBM (Wang et al., 2025), CLEAR (Dikter et al., 2024), and DOT-CBM (Xie et al., 2025). Besides, following (Gao et al., 2024; Wang et al., 2025), we also compare black-box models (He et al., 2015; Dosovitskiy et al., 2021) and multi-modal backbones (Radford et al., 2021; Wang et al., 2022; Zhang et al., 2025).

To account for the class imbalance prevalent in these benchmarks, we employ both Accuracy (ACC) and Balanced Macro Average Accuracy (BMAC) for a comprehensive evaluation. For implementation details, please refer to [Appendix B](#).

Table 1: Performance comparison (ACC % and BMAC %) on multiple medical datasets. We evaluate our model against various zero-shot, black-box, and explainable models. Best results are highlighted in **bold**. Gains are compared within Explainable methods.

Model	ISIC		NCT		IDRID		BUSI		Retina		SIIM		Cardio		CMMB	
	ACC	BMAC														
<i>Zero-shot</i>																
CLIP [ICML 2021]	29.88	21.32	26.67	26.71	29.84	25.92	43.85	37.85	18.33	25.00	41.01	22.15	54.81	49.12	27.10	34.00
MedCLIP [EMNLP 2022]	13.68	15.31	9.57	12.05	16.86	19.57	27.44	43.19	17.50	25.42	42.34	41.01	45.94	46.66	27.10	30.72
BiomedCLIP [NEJM AI 2025]	59.83	24.47	40.51	40.39	39.15	30.31	29.36	36.45	53.33	38.33	39.88	20.92	49.13	46.70	52.90	50.00
<i>Black-box</i>																
ResNet50 [CVPR 2016]	83.53	76.53	92.12	91.34	54.38	55.88	76.41	75.84	78.33	77.50	87.97	76.21	81.51	81.51	74.59	60.46
ViT Base [ICLR 2021]	90.01	84.14	93.25	92.73	58.07	54.70	80.25	83.63	83.33	76.66	83.56	74.15	79.60	79.61	74.77	60.35
<i>Explainable</i>																
LaBo [CVPR 2023]	79.20	80.83	91.73	91.62	50.77	54.17	84.01	85.98	72.60	73.83	74.13	72.16	73.48	73.73	70.78	65.59
PCBM [ICLR 2023]	85.91	81.76	91.77	91.18	54.36	58.85	84.64	88.91	66.67	69.17	80.02	75.68	76.43	76.41	69.24	66.68
COOP-CBM [Nips 2023]	86.82	79.25	93.43	93.78	61.22	50.41	89.61	89.73	85.00	80.83	86.14	79.81	80.57	80.58	77.28	64.25
LF-CBM [ICLR 2023]	83.55	78.46	87.92	87.77	60.59	56.97	76.77	75.77	73.33	70.83	77.62	71.59	75.95	75.95	74.75	60.18
Explid [MICCAI 2024]	88.72	82.42	95.29	94.73	63.26	63.61	87.17	87.37	83.33	81.67	85.70	78.90	78.95	78.94	76.74	60.48
MVP-CBM [IJCAI 2025]	87.72	80.35	97.90	97.89	65.38	57.78	89.74	91.45	85.00	83.33	84.89	78.95	80.29	80.29	75.84	56.15
CLEAR [WACV 2025]	86.25	81.11	89.05	86.86	56.54	58.33	83.85	83.33	72.89	70.56	78.26	70.12	78.22	78.18	73.35	61.23
DOT-CBM [CVPR 2025]	86.55	81.37	90.15	91.51	58.45	59.12	85.23	84.10	74.59	71.88	79.52	76.48	77.15	77.10	71.15	62.98
IVQ-CBM (Ours)	90.11	86.22	99.90	99.88	67.35	73.06	93.59	95.38	88.33	85.83	88.03	81.91	82.01	82.01	79.25	69.70
+Δ	+1.39	+3.80	+2.00	+1.99	+1.97	+9.45	+3.85	+3.93	+3.33	+2.50	+1.89	+2.10	+1.44	+1.43	+1.97	+3.02

Table 2: Performance comparison (ACC % and BMAC %) on multiple benchmark datasets. We evaluate our model against various state-of-the-art methods. Best results are highlighted in **bold**. Gains are compared against the second-best method.

Model	CIFAR-10		CIFAR-100		CUB		Places365		ImageNet	
	ACC	BMAC								
<i>LaBo [CVPR 2023]</i>										
LaBo [CVPR 2023]	80.23	79.15	60.17	59.95	69.88	69.72	39.67	39.41	68.04	67.88
PCBM [ICLR 2023]	84.61	84.49	63.22	63.07	72.36	72.19	41.13	40.99	70.14	69.97
COOP-CBM [Nips 2023]	85.17	84.99	64.21	64.03	73.06	72.87	42.19	42.01	71.23	71.09
LF-CBM [ICLR 2023]	82.94	82.78	61.89	61.73	71.42	71.22	40.33	40.15	69.46	69.21
Explid [MICCAI 2024]	86.03	85.88	64.91	64.78	74.08	73.91	43.07	42.89	71.93	71.77
MVP-CBM [IJCAI 2025]	86.72	86.54	65.48	65.30	74.63	74.45	43.81	43.66	72.29	72.15
CLEAR [WACV 2025]	83.77	83.59	62.83	62.61	71.84	71.69	40.92	40.75	68.81	68.66
DOT-CBM [CVPR 2025]	84.38	84.19	63.45	63.28	72.29	72.11	41.76	41.53	69.31	69.17
IVQ-CBM (Ours)	88.14	87.91	67.12	66.88	75.91	75.68	45.54	45.32	73.42	73.23
+Δ	+1.42	+1.37	+1.64	+1.58	+1.28	+1.23	+1.73	+1.66	+1.13	+1.08

4.1 BASIC EXPERIMENTS

Benchmark Comparison. As demonstrated in our experiments in Table 1, our method consistently outperforms all baselines across the entire suite of medical datasets, illustrating its robust capabilities

378 Table 3: Ablation experiments showing both ACC and BMAC metrics for each experimental setup. The final
 379 rows display the performance gains ($+\Delta$ in red) of our full model over the second-best configuration.

Components		Metric	Datasets							
			ISIC	NCT	IDRID	BUSI	Retina	SIIM	Cardio	CMMD
IVQ	Magnet	ACC	80.88	95.23	57.14	88.46	75.00	85.72	80.21	74.59
✗	✓	BMAC	84.84	94.92	45.27	87.37	69.16	78.45	80.21	52.55
✓	✗	ACC	89.42	96.23	65.38	92.31	83.33	86.47	81.11	77.63
✓	✗	BMAC	82.85	95.61	61.25	91.15	80.00	80.49	81.11	66.81
✓	✓	ACC	90.11 ($+\Delta$ 0.69)	99.90 ($+\Delta$ 3.67)	67.35 ($+\Delta$ 1.97)	93.59 ($+\Delta$ 1.28)	88.33 ($+\Delta$ 5.00)	88.03 ($+\Delta$ 1.56)	82.01 ($+\Delta$ 0.90)	79.25 ($+\Delta$ 1.62)
		BMAC	86.22 ($+\Delta$ 1.38)	99.88 ($+\Delta$ 4.27)	73.06 ($+\Delta$ 11.81)	95.38 ($+\Delta$ 4.23)	85.83 ($+\Delta$ 5.83)	81.91 ($+\Delta$ 1.42)	82.01 ($+\Delta$ 0.90)	69.70 ($+\Delta$ 2.89)

391
 392 under diverse diagnostic conditions. In particular, our approach surpasses traditional black-box pre-
 393 dictive models, demonstrating that it maintains high diagnostic performance while simultaneously
 394 providing interpretability. This addresses the critical performance-interpretability trade-off that has
 395 been a significant challenge in previous works (Zarlenaga et al., 2022).

396 To further validate the scalability and generalization of our framework beyond the medical domain,
 397 we extended our evaluation to standard broad-domain benchmarks. As presented in Table 2, IVQ-
 398 CBM achieves superior performance across all five datasets, ranging from fine-grained classification
 399 tasks like CUB to large-scale challenges such as ImageNet. Notably, our method demonstrates con-
 400 sistent gains over the strongest baselines (e.g., +1.64% on CIFAR-100 and +1.13% on ImageNet),
 401 confirming that the benefits of implicit quantization scale effectively to complex, high-dimensional
 402 visual distributions.

403 Furthermore, to investigate the underlying mechanism of these performance gains, we analyzed the
 404 feature rank dynamics throughout training. Figure 4 and Figure 5 present the rank evolution across
 405 medical and general benchmarks, respectively. The results reveal a fundamental distinction between
 406 our method and prior arts. While competing methods, particularly DOT-CBM (Xie et al., 2025)
 407 and MVP-CBM, suffer from varying degrees of representational collapse, our approach consistently
 408 maintains a high and stable feature rank across all datasets. This issue of collapse is notably aggra-
 409 vated on complex datasets like ImageNet, as shown in Figure 5, where the feature ranks of baseline
 410 models exhibit a drastic decline. This provides compelling evidence that IVQ acts as a robust reg-
 411 ularizer that effectively prevents the degeneration of the feature space. By preserving high-rank
 412 and diverse representations, this structural advantage directly correlates with the superior and more
 413 robust downstream performance observed in both Table 1 and Table 2.

414 **Ablation Study.** Our ablation study (Table 3) confirms that both the IVQ and Magnet modules are
 415 integral to performance. IVQ provides the most significant boost, especially on the BMAC metric
 416 for imbalanced datasets like IDRID (+11.81). Removing the Magnet module and reverting to a
 417 standard [CLS] token baseline leads to a notable performance drop. This indicates that relying on
 418 a single global feature vector is an oversimplification of the image’s content. While this approach
 419 may suffice for coarse-grained classification, it is inadequate for complex scenes requiring fine-
 420 grained analysis, such as localizing small or scattered targets—a common challenge in medical
 421 imaging (Chen et al., 2021). Furthermore, we find that IVQ’s mechanism is linked to preventing
 422 *representation collapse* (Figure 6). Models without IVQ suffer from rank collapse (dashed lines),
 423 whereas our method maintains a high, stable feature rank (solid lines). This shows IVQ acts as a
 424 powerful regularizer, ensuring diverse and robust feature learning.

425 4.2 EXTENSIVE EXPERIMENTS

426
 427 **Vector Quantization versus Implicit Vector Quantization.** As previously established, an inher-
 428 ent many-to-many correspondence exists between visual patches and textual concepts, with each
 429 patch often encoding multi-faceted semantic information. Standard VQ conflicts with this principle
 430 (Van Den Oord et al., 2017b). Its use of a hard argmin operation maps each patch to a single,
 431 nearest codebook vector, which forces the collapse of a patch’s rich information into a discrete rep-
 432 resentation. Consequently, only these quantized features are passed forward to the magnet module,

432 Table 4: Ablation study of different representation quantization methods on various medical datasets. The table
 433 compares performance in terms of Classification BMAC and Concept BMAC. The improvement of our implicit
 434 method over the explicit baseline is shown in parentheses ($+\Delta$).

Dataset	Explicit Quantization		Implicit Quantization (ours)	
	Classification BMAC	Concept BMAC	Classification BMAC	Concept BMAC
ISIC	51.47	22.22	86.22 ($+\Delta$ 34.75)	83.88 ($+\Delta$ 61.66)
Cardio	60.61	53.30	82.01 ($+\Delta$ 21.40)	80.25 ($+\Delta$ 26.95)
BUSI	57.28	37.48	95.38 ($+\Delta$ 38.10)	71.02 ($+\Delta$ 33.54)
SIIM	50.00	50.00	81.91 ($+\Delta$ 31.91)	80.15 ($+\Delta$ 30.15)
CMMMD	50.35	50.00	69.70 ($+\Delta$ 19.35)	66.66 ($+\Delta$ 16.66)
IDRID	23.75	50.85	73.06 ($+\Delta$ 49.31)	59.48 ($+\Delta$ 8.63)

445 Table 5: Performance comparison of our model and other representation regularization techniques across
 446 datasets. Gains ($+\Delta$) and losses ($-\Delta$) are shown relative to the best-performing alternative technique.

Technique	SIIM		ISIC		BUSI	
	ACC	BMAC	ACC	BMAC	ACC	BMAC
Barlow Twins (Zbontar et al., 2021)	86.39	79.17	87.62	81.16	91.02	88.81
Spectral Regularization (Yoshida & Miyato, 2017)	85.64	80.84	90.21	84.74	92.30	91.98
Gram Loss (Siméoni et al., 2025)	84.56	74.07	76.64	59.83	84.61	82.68
IVQ (Ours)	88.03 ($+1.64$)	81.91 ($+1.07$)	90.11 (-0.10)	86.22 ($+1.48$)	93.59 ($+1.29$)	95.38 ($+3.40$)

456
 457 discarding other relevant visual attributes and violating the many-to-many relationship, leading to
 458 the critical **information bottleneck** issue. In contrast, our IVQ is designed to resolve this issue. It
 459 retains the quantization objective solely as a regularizer, encouraging each raw patch feature to align
 460 with its nearest prototype. Crucially, this allows the original, high-fidelity feature vector to be used
 461 in the forward pass for the magnet module. This process distills the core conceptual information
 462 from the patch, enabling a more effective concept alignment. Results are summarized in [Table 4](#),
 463 revealing that IVQ substantially outperforms the explicit quantization across all six datasets, on both
 464 Classification and Concept BMAC metrics.

465
 466 **Representation Regularization Techniques.** Several representation regularization techniques
 467 have been proposed to mitigate feature rank collapse, particularly in SSL. We benchmark our pro-
 468 posed IVQ against three prominent methods: explicit de-correlation via Barlow Twins (Zbontar
 469 et al., 2021), Spectral regularization (Yoshida & Miyato, 2017), and Gram Loss (Siméoni et al.,
 470 2025). As shown in [Table 5](#), IVQ consistently outperforms these general-purpose regularization
 471 techniques across most metrics, yielding significant gains over the strongest baseline.

472 A critical question raises: is a higher feature rank directly correlated with superior CBM per-
 473 formance? An analysis of feature rank dynamics, presented in [Figure 7](#), reveals a more nuanced re-
 474 lationship. While methods like Barlow Twins and Spectral regularization often maintain a higher
 475 feature rank than IVQ, particularly on the ISIC and BUSI datasets, this elevated rank does not trans-
 476 late to better downstream performance, suggesting a form of **over-regularization**. We attribute this
 477 to a key distinction: unlike general-purpose methods that indiscriminately maximize feature diver-
 478 sity, IVQ is tailored to foster the **meaningful, structured diversity** required by CBMs by aligning
 479 features with a set of learnable prototypes.

480
 481 **Analysis of Codebook Size** The IVQ codebook dynamically aligns patch features with a set of
 482 learnable prototypes, which ensures feature diversity while distilling core visual information and
 483 avoiding the bottleneck of conventional VQ. This raises a key question regarding the optimal size of
 484 the codebook, M , in relation to the number of textual concepts, K . To investigate this, we conduct
 485 an ablation study, setting the codebook size to various multiples of the concept count (i.e., $M = \alpha K$
 for $\alpha \in \{20, 10, 5, 1\}$), as well as a baseline with a single shared prototype ($M = 1$).

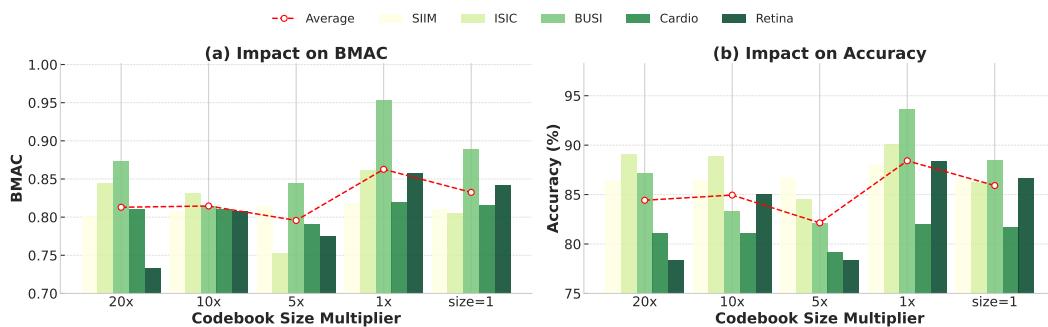


Figure 3: Performance (ACC & BMAC) across various codebook sizes. The size is defined as a multiple (\times) of the number of textual concepts, K .

As illustrated in Figure 3, the model’s performance is robust across a range of oversized codebooks ($20\times$, $10\times$, and $5\times$), but we observe a distinct peak in both average ACC and BMAC when the codebook size is set equal to the number of textual concepts ($M = K$). This setting achieves the highest average BMAC and Accuracy across all datasets. We hypothesize that setting $M = K$ encourages a **one-to-one mapping** between the learned visual prototypes and the predefined textual concepts, fostering a more structured and semantically aligned representation space. It provides strong evidence for the critical role of our IVQ as a bridge between visual patches and textual concepts, acting as a system of visual semantic anchors. These results suggest that aligning the codebook’s capacity with the task’s conceptual granularity is the optimal strategy.

Visualization of CodeBook in IVQ The IVQ continuously distills visual information for each concept during training. To qualitatively evaluate the knowledge captured within the final codebook, we visualize the index maps of our learned prototypes on a representative mammogram from the CMMMD dataset, as shown in Figure 8a.

The resulting mapping demonstrates a highly logical process that mirrors clinical reasoning. The prototype for Mass Margin (light green) precisely delineates the lesion’s contour, while those for Mass Shape (cyan) and Calcification Features (blue) correspond to its internal characteristics. Crucially, the prototype for Associated Features (dark blue) extends its focus beyond the lesion’s border, probing the surrounding parenchyma for signs of structural distortion—a key indicator of malignancy. This structured, multi-faceted assessment validates that our codebook has learned semantically meaningful and clinically relevant concept representations (For a more detailed visual analysis, please refer to the appendix D).

5 CONCLUSION

In this work, we propose **IVQ-CBM**, which explicitly models the many-to-many relationship while addressing representation collapse. Our method features two key components. IVQ, which uses a learnable codebook prior to anchor visual patches, and Magnet Attention, which aggregates these patches into semantically coherent visual concepts aligned with textual definitions. Extensive experiments demonstrate that IVQ-CBM achieves superior performance over baselines without sacrificing interpretability, with ablation studies validating each component’s contribution. Our analysis reveals that IVQ circumvents the hard information bottleneck of direct VQ and, unlike general regularization methods, fosters a *meaningful* feature diversity that is more effective than indiscriminately maximizing a mathematical objective. Visualizations confirm that our approach yields high-quality, interpretable visual concept representations that are consistent with their textual concepts, resulting in a more faithful and robust form of interpretability for CBMs.

REPRODUCIBILITY STATEMENT

To ensure reproducibility, we release the source code in the supplementary materials. All datasets used in our experiments are either publicly available; the implementation details, including model architectures, hyper-parameters, and optimization settings, are described in section 4 and Appendix B.

540 For baselines, we rely on publicly released implementations and adapt them with the same pre-
 541 processing pipeline as described in [section 4.1](#). We hope these materials enable the community to
 542 faithfully reproduce our results and extend our approach.
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APPENDIX

In this section, we present additional implementation details, experiment results, theoretical analysis, pseudo code, and supplements. The content structure is outlined as follows:

- Section A - Theoretical Analysis
 - Section A.1 - Motivation: The Fundamental Limitations of a Single Global Feature
 - Section A.2 - Proof of Intrinsic Many-to-Many Coupling
 - Section A.3 - Theoretical Analysis: Optimization Dynamics and Rank Preservation
 - Section A.4 - Theoretical Analysis for Gradient Convergence
- Section B - Implementation Details
- Section C - Feature Rank Dynamics
- Section D - Visualization of Codebook in IVQ
- Section E - Visualization of Codebook in VQ
- Section F - Visualization Analysis With Baselines
- Section G - Results with Other Multi-Modal Backbone
- Section H - Statement on the Use of Large Language Models
- Section I - Pseudocode of IVQ-CBM
- Section J - Quantitative Interpretability and Casual Faithfulness
- Section K - Analysis of Information Leakage and Effective Concept Learning
- Section L - Sensitivity Analysis of Commitment Cost Parameter

A THEORETICAL ANALYSIS

A.1 MOTIVATION: THE FUNDAMENTAL LIMITATIONS OF A SINGLE GLOBAL FEATURE

A prevailing and influential paradigm in the evolution of Concept Bottleneck Models is the use of a single global feature from a pre-trained vision model, such as CLIP, as the sole representation of an input image. Specifically, these models typically rely on the final [CLS] token from a Vision Transformer (ViT) or the feature vector generated by a Global Average Pooling (GAP) layer in a Convolutional Neural Network (CNN) (He et al., 2015). The implicit assumption underpinning this approach is that a single high-dimensional vector (e.g., $D = 768$) can sufficiently and comprehensively encapsulate all semantic information relevant to downstream tasks. In other words, it posits that this single, condensed vector is a complete basis for identifying all pertinent concepts and, ultimately, the final class label.

However, we argue that this seemingly efficient simplification is, in fact, an *illusion of sufficiency* that conceals fundamental flaws. While it may suffice for simple, object-centric classification tasks, its limitations are starkly exposed when confronted with visually complex scenes that demand fine-grained understanding.

Our central thesis is that the reliance on a single global feature vector is an **untenable design simplification** for building robust, interpretable, and broadly applicable CBMs. This simplification is particularly fragile in scenarios where:

- The image contains multiple, spatially distinct objects or concepts.
- The critical differentiating information lies in subtle, local details or textures.
- The key features are inherently distributed or non-centralized.

This argument is not speculative but is grounded in the unavoidable theoretical limitations inherent to the mechanisms that generate this global vector. We prove this by deconstructing its three fatal flaws.

810 **1. Irreversible Loss of Spatial Information.** The generation of a single global vector is, by its
 811 very nature, a process that destroys spatial structure. For a CNN-based GAP layer, the mechanism
 812 averages a feature map of size $H \times W \times D$ across its spatial dimensions to produce a $1 \times 1 \times D$
 813 vector. This operation is mathematically *permutation-invariant*; as long as the set of local features
 814 remains the same, their spatial arrangement can be arbitrarily altered with little to no change in the
 815 resulting global vector. This is analogous to calculating the word frequency of a document while
 816 discarding the sentences and paragraphs. We know *what* content is present, but we have permanently
 817 lost *how* it is organized. Consequently, any task requiring answers to "where?" or an understanding
 818 of spatial relationships is impossible for a model that has discarded all coordinate information.

819 For the Transformer-based [CLS] token, while its computation involves a spatially-aware self-
 820 attention mechanism, the process is ultimately one of *aggregation and summarization*. The final
 821 [CLS] output is an abstract vector that has encoded spatial relationships into its dimensions, but the
 822 explicit, original topological structure is lost (Park & Kim, 2022). The attention maps exist during
 823 computation, but the final vector itself does not retain this map. **Conclusion:** A single global vector
 824 actively discards the two-dimensional structure of an image, which is its first fatal flaw (Yu et al.,
 825 2022).

826
 827 **2. The Information Bottleneck and Feature Suppression.** A vector of fixed dimensionality has
 828 a finite capacity for information, creating a natural bottleneck (Butakov et al., 2024). Within an
 829 image, different regions, objects, and textures must compete for representation within this fixed
 830 bandwidth. In this process of *feature competition*, strong signals (from large, prominent objects)
 831 will disproportionately dominate the final vector's representation, while weak signals (from small
 832 or subtle objects) are easily averaged out or *suppressed* (Li et al., 2023). Consider a thought experi-
 833 ment: a high-resolution CT scan where 99.9% of the image consists of healthy lung tissue (a strong
 834 signal) and only 0.1% contains a small, early-stage pulmonary nodule (a weak signal). During the
 835 global aggregation process, the features representing healthy tissue will overwhelm the vector, making
 836 it nearly impossible for the faint but critical signal from the nodule to survive this democratic
 837 aggregation (Guo et al., 2019). **Conclusion:** The limited capacity of a single global vector forces
 838 a lossy compression that systematically sacrifices the fine-grained or low-prevalence information
 839 critical for complex tasks.

840
 841 **3. Representational Failure for Multiple Instances and Concepts.** The core promise of a CBM
 842 is a clear mapping from image features to concepts. A single global vector is powerless to man-
 843 age this when "many-to-many" relationships are required. When multiple independent semantic
 844 concepts coexist in an image (e.g., "striped texture," "pointed ears," and "furry texture"), a single
 845 vector is forced to *entangle* these disparate pieces of information (Li et al., 2024). This entanglement
 846 leads to severe *representational ambiguity*. An activation in a 21 dimension might represent concept
 847 A, concept B, or an inseparable combination of A and C. This fundamentally violates the goal of
 848 CBMs to be interpretable and intervenable. An ideal concept bottleneck should have distinct "chan-
 849 nels" corresponding to disentangled concepts (Xie et al., 2025). For example, an intervention on the
 850 "pointed ears" concept becomes meaningless if its representation is coupled with the "furry texture"
 851 concept, as we cannot modify one without affecting the other. **Conclusion:** To model multiple con-
 852 cepts independently and clearly, a model requires access to multiple, separable visual features prior
 853 to the concept alignment stage. A single global vector cannot meet this fundamental requirement.

854 In summary, drawing from the current paradigm of CBMs that rely on a single global feature, we
 855 have proven through theoretical analysis that this is a fundamentally flawed simplification. Its three
 856 fatal flaws—the loss of spatial information, the creation of an information bottleneck, and the failure
 857 to represent multiple concepts clearly—are inherent to its generation mechanism. This provides a
 858 solid and compelling theoretical foundation for our proposed paradigm: establishing a many-to-
 859 many mapping between local image features (patches) and semantic concepts.

860 A.2 PROOF OF INTRINSIC MANY-TO-MANY COUPLING

861
 862 **Proposition 1.** *Within the proposed IVQ-CBM framework, (i) each learned Visual Concept in-
 863 evitably depends on multiple visual patch embeddings, and (ii) each visual patch embedding in-
 864 evitably contributes to multiple Visual Concepts.*

864 *Proof.* We prove the two parts of the proposition separately.
 865

866 1. FORMAL DEFINITIONS AND NOTATION
 867

868 We adopt the notation from the method section.
 869

870 **Visual Patch Embeddings** $\mathbf{Z}_p = [\mathbf{z}_1, \dots, \mathbf{z}_L] \in \mathbb{R}^{L \times D}$ are the patch embeddings from the ViT
 871 encoder \mathcal{E}_v .
 872

873 **Concept Queries** $\mathbf{Q} = [\mathbf{q}_1, \dots, \mathbf{q}_K]^\top \in \mathbb{R}^{K \times D}$ is the matrix of learnable concept queries.
 874

875 **Soft Assignment Matrix** $\mathbf{A} \in \mathbb{R}^{L \times K}$, where its element A_{jk} represents the soft-assignment
 876 weight of patch j to concept k :

$$A_{jk} = \frac{\exp(-\|\mathbf{z}_j - \mathbf{q}_k\|_2^2)}{\sum_{k'=1}^K \exp(-\|\mathbf{z}_j - \mathbf{q}_{k'}\|_2^2)}.$$

877 **Visual Concepts** $\mathbf{M} = [\mathbf{m}_1, \dots, \mathbf{m}_K]^\top = \mathbf{A}^\top \mathbf{Z}_p \in \mathbb{R}^{K \times D}$ is the matrix of aggregated Visual
 878 Concepts. The k -th visual concept is given by $\mathbf{m}_k = \sum_{j=1}^L A_{jk} \mathbf{z}_j$.
 879

880 **Concept Prediction** The activation score for concept k , denoted v_k , is the cosine similarity between
 881 the visual concept \mathbf{m}_k and its corresponding textual concept embedding τ_k , i.e., $v_k = \frac{\mathbf{m}_k \cdot \tau_k}{\|\mathbf{m}_k\| \|\tau_k\|}$. The final prediction is $\hat{c}_k = \sigma(v_k)$, where σ is the sigmoid function for the BCE
 882 loss.
 883

884 2. PROOF: “ONE CONCEPT–MULTIPLE PATCHES” IS ALMOST CERTAIN
 885

886 This proposition states that for any given Visual Concept \mathbf{m}_k , its final representation and subsequent
 887 prediction \hat{c}_k are influenced by multiple patch embeddings.
 888

889 **Lemma 1** (Sufficiency). *Let A_{jk} be the soft-assignment weight for patch j and concept k . If there
 890 exist two distinct patch indices $i \neq j$ such that their assignment weights to concept k are non-zero
 891 (i.e., $A_{ik} > 0$ and $A_{jk} > 0$), then the concept prediction \hat{c}_k simultaneously depends on both patch
 892 embeddings \mathbf{z}_i and \mathbf{z}_j , as demonstrated by their non-zero gradients:*
 893

$$\frac{\partial \hat{c}_k}{\partial \mathbf{z}_i} \neq 0 \quad \text{and} \quad \frac{\partial \hat{c}_k}{\partial \mathbf{z}_j} \neq 0.$$

894 *Proof of Lemma.* We apply the chain rule to compute the gradient of the concept prediction \hat{c}_k with
 895 respect to a patch embedding \mathbf{z}_j . Since $\frac{\partial \hat{c}_k}{\partial \mathbf{z}_j} = \sigma'(v_k) \frac{\partial v_k}{\partial \mathbf{z}_j}$ and $\sigma'(v_k) \neq 0$ almost everywhere, we
 896 only need to analyze the gradient of the activation score, $\frac{\partial v_k}{\partial \mathbf{z}_j}$.
 897

$$\frac{\partial v_k}{\partial \mathbf{z}_j} = \frac{\partial v_k}{\partial \mathbf{m}_k} \frac{\partial \mathbf{m}_k}{\partial \mathbf{z}_j}.$$

898 The visual concept $\mathbf{m}_k = \sum_{l=1}^L A_{lk} \mathbf{z}_l$. The derivative of \mathbf{m}_k with respect to \mathbf{z}_j involves two
 899 components, as the assignment weights A_{lk} also depend on \mathbf{z}_j :
 900

$$\frac{\partial \mathbf{m}_k}{\partial \mathbf{z}_j} = \underbrace{A_{jk} \cdot \mathbf{I}}_{\text{Direct Term}} + \underbrace{\sum_{l=1}^L \frac{\partial A_{lk}}{\partial \mathbf{z}_j} \otimes \mathbf{z}_l}_{\text{Attention Term}},$$

901 where \mathbf{I} is the identity matrix and \otimes is the outer product. The *Direct Term* $A_{jk} \cdot \mathbf{I}$ is non-zero as
 902 long as the assignment weight A_{jk} is non-zero. This term captures the direct contribution of patch
 903 \mathbf{z}_j to the weighted average. The *Attention Term* captures the indirect influence of changing \mathbf{z}_j on
 904 the attention weights of all other patches and is generally non-zero.
 905

906 Since A_{jk} is strictly positive (due to the exponential function in softmax), the Direct Term ensures
 907 that $\frac{\partial \mathbf{m}_k}{\partial \mathbf{z}_j}$ is non-zero. The gradient $\frac{\partial v_k}{\partial \mathbf{m}_k}$ is also non-zero in general. Therefore, the total gradient $\frac{\partial \hat{c}_k}{\partial \mathbf{z}_j}$
 908 is non-zero. This holds for any patch j with a non-zero assignment weight, proving the lemma. \square
 909

918 **Probability = 1 Argument.** The condition of the lemma, $A_{ik} > 0$ and $A_{jk} > 0$, is certain to hold.
 919 The assignment weight A_{jk} is calculated as $\exp(-\|\mathbf{z}_j - \mathbf{q}_k\|_2^2)$ divided by a sum of such terms.
 920 Since the squared Euclidean distance is finite and the exponential function is strictly positive for all
 921 finite inputs, every assignment weight A_{jk} is strictly greater than zero for any $j \in \{1, \dots, L\}$ and
 922 $k \in \{1, \dots, K\}$. Consequently, every patch has a non-zero influence on every concept. The “one
 923 concept–multiple patches” relationship is not just almost certain; it is a structural certainty of the
 924 Magnet Attention mechanism.

925 **3. PROOF: “ONE PATCH–MULTIPLE CONCEPTS” IS ALMOST CERTAIN**

926 This proposition states that a single patch embedding \mathbf{z}_j will meaningfully contribute to the forma-
 927 tion of multiple Visual Concepts.

928 **Gradient-based Argument.** Consider the update to a patch embedding \mathbf{z}_j during backpropaga-
 929 tion, driven by the concept alignment loss $\mathcal{L}_{\text{concept}} = \sum_{k=1}^K \mathcal{L}_{\text{BCE}}(\hat{c}_k, c_k)$. The gradient of the loss
 930 with respect to \mathbf{z}_j is:

$$\frac{\partial \mathcal{L}_{\text{concept}}}{\partial \mathbf{z}_j} = \sum_{k=1}^K \frac{\partial \mathcal{L}_{\text{concept}}}{\partial \hat{c}_k} \frac{\partial \hat{c}_k}{\partial \mathbf{z}_j} = \sum_{k=1}^K \underbrace{\left(\frac{\hat{c}_k - c_k}{\hat{c}_k(1 - \hat{c}_k)} \right)}_{\text{Error signal for concept } k} \underbrace{\frac{\partial \hat{c}_k}{\partial \mathbf{z}_j}}_{\text{Influence of patch } j \text{ on } k}.$$

931 As established in the previous section, the influence term $\frac{\partial \hat{c}_k}{\partial \mathbf{z}_j}$ is non-zero for all concepts k . There-
 932 fore, if the model has a non-zero prediction error for more than one concept (i.e., $\hat{c}_k - c_k \neq 0$ for
 933 multiple k), the total gradient received by patch \mathbf{z}_j will be a sum of contributions from all those
 934 concepts. Since natural images typically contain features relevant to multiple concepts, the SGD
 935 update will pull \mathbf{z}_j in a direction that is a composite of gradients from multiple concepts, making
 936 patch \mathbf{z}_j influential for all of them.

937 **Softmax Competition Argument.** We can formalize the argument that a single patch is unlikely to
 938 contribute to only one concept by quantitatively analyzing the conditions required for the assignment
 939 distribution to become nearly one-hot.

940 Let’s start by introducing a temperature parameter $\tau > 0$ into the softmax function, which controls
 941 the sharpness of the output distribution. The assignment weight of patch j to concept k is given by:

$$A_{jk} = \frac{\exp(-\|\mathbf{z}_j - \mathbf{q}_k\|_2^2/\tau)}{\sum_{k'=1}^K \exp(-\|\mathbf{z}_j - \mathbf{q}_{k'}\|_2^2/\tau)}.$$

942 For the original formulation, we can simply consider $\tau = 1$. A “one-hot” assignment, where patch j
 943 contributes almost exclusively to a single concept, means that for some concept k^* , its weight A_{jk^*}
 944 approaches 1.

945 Let k^* be the index of the concept query closest to the patch embedding \mathbf{z}_j :

$$k^* = \arg \min_{k \in \{1, \dots, K\}} \|\mathbf{z}_j - \mathbf{q}_k\|_2^2.$$

946 To quantify the significance of this closest distance, we define the **minimum distance margin** Δ_{\min}
 947 for patch \mathbf{z}_j as the difference between the squared distance to the second-closest query and the
 948 closest one:

$$\Delta_{\min} \triangleq \min_{k' \neq k^*} (\|\mathbf{z}_j - \mathbf{q}_{k'}\|_2^2 - \|\mathbf{z}_j - \mathbf{q}_{k^*}\|_2^2).$$

949 A large $\Delta_{\min} \geq 0$ indicates that \mathbf{z}_j has a clear “winner” concept query, while a small Δ_{\min} suggests
 950 high competition. Now, we establish a lower bound for the maximum assignment weight A_{jk^*} :

$$A_{jk^*} = \frac{1}{1 + \sum_{k' \neq k^*} \exp\left(-\frac{\|\mathbf{z}_j - \mathbf{q}_{k'}\|_2^2 - \|\mathbf{z}_j - \mathbf{q}_{k^*}\|_2^2}{\tau}\right)}.$$

972 By definition, $\|\mathbf{z}_j - \mathbf{q}_{k'}\|_2^2 - \|\mathbf{z}_j - \mathbf{q}_{k^*}\|_2^2 \geq \Delta_{\min}$ for any $k' \neq k^*$. This allows us to bound the
 973 sum in the denominator, yielding the inequality:
 974

$$975 \quad A_{jk^*} \geq \frac{1}{1 + (K-1)e^{-\Delta_{\min}/\tau}}.$$

$$976$$

977 This inequality provides a precise condition for a one-hot assignment. For A_{jk^*} to be nearly
 978 1 (e.g., $A_{jk^*} \geq 1 - \epsilon$), the margin-to-temperature ratio Δ_{\min}/τ must be large, specifically
 979 $\Delta_{\min} \geq \tau \log(\frac{K-1}{\epsilon})$. In other words, a patch can only be exclusively assigned to one concept
 980 if its embedding \mathbf{z}_j is **geometrically well-separated** from all but one concept query.
 981

982 Such a large margin is geometrically improbable in high-dimensional spaces due to the **concen-**
 983 **tration of measure phenomenon** (Vershynin, 2018), which states that distances between random
 984 points tend to be tightly clustered. It is far more likely that \mathbf{z}_j will be reasonably close to several
 985 queries, leading to a small Δ_{\min} and thus a distributed (non-sparse) set of assignment weights. The
 986 soft nature of the attention mechanism, combined with these geometric properties, ensures that each
 987 patch almost certainly contributes to multiple concepts.
 988

4. CONCLUSION

990 The Magnet Attention mechanism, by its design, establishes a dense, many-to-many coupling be-
 991 between patch embeddings and visual concepts.
 992

- 993 **1. One Concept to Multiple Patches:** This occurs with structural certainty due to the nature
 994 of the soft attention mechanism where all weights are non-zero.
 995
- 996 **2. One Patch to Multiple Concepts:** This is a highly probable outcome under standard train-
 997 ing conditions. The competitive nature of the softmax function makes a one-hot assignment
 998 (where one patch contributes to only one concept) an unstable and non-generic solution in
 999 a high-dimensional space. Furthermore, the training dynamics, driven by multi-concept
 1000 error signals, actively steer patch embeddings to be useful for multiple concepts.

1001 Therefore, the patch-concept mapping in the proposed model is intrinsically many-to-many, provid-
 1002 ing a robust foundation for learning comprehensive and interpretable visual concepts. \square
 1003

1004 A.3 THEORETICAL ANALYSIS: OPTIMIZATION DYNAMICS AND RANK PRESERVATION

1005 In this section, we provide a formal analysis of how the optimization dynamics of the proposed IVQ
 1006 loss explicitly counteract representational collapse and preserve the rank of the feature space.
 1007

1008 **1. Optimization Dynamics as a Restoring Force.** Recall the commitment loss component of the
 1009 IVQ objective defined in Eq. 4:
 1010

$$1011 \quad \mathcal{L}_{\text{commit}} = \beta \sum_{j=1}^L \|\mathbf{z}_j - \text{sg}(\mathbf{c}_{k_j})\|_2^2, \quad (10)$$

$$1012$$

1013 where $\mathbf{z}_j \in \mathbb{R}^D$ is the j -th patch feature, and \mathbf{c}_{k_j} is its nearest neighbor in the codebook \mathcal{C}_{vq} . During
 1014 backpropagation, the gradient of this loss with respect to a specific patch feature \mathbf{z}_j is given by:
 1015

$$1016 \quad \nabla_{\mathbf{z}_j} \mathcal{L}_{\text{commit}} = 2\beta(\mathbf{z}_j - \mathbf{c}_{k_j}). \quad (11)$$

$$1017$$

1018 This gradient can be interpreted physically as a *restoring force* in the high-dimensional feature space.
 1019 It actively pulls every patch embedding \mathbf{z}_j towards its assigned semantic prototype \mathbf{c}_{k_j} . Unlike stan-
 1020 dard contrastive losses that primarily push features apart, this dynamic acts as a structured gravi-
 1021 tational pull, clustering the continuous distribution of patch features into compact regions centered
 1022 around the learned prototypes.
 1023

1026 **2. Geometric Interpretation and Rank Lower Bound.** Representational collapse manifests as a
 1027 rapid decay in the singular values of the feature matrix $Z_p \in \mathbb{R}^{L \times D}$, causing features to degenerate
 1028 into a low-dimensional subspace (i.e., $\text{rank}(Z_p) \ll K$). The IVQ mechanism imposes a geometric
 1029 constraint that counteracts this degeneracy.

1030 Empirically, as shown in our ablation study ($M = K$) and UMAP visualizations (Figure 9), the
 1031 codebook prototypes $\{c_1, \dots, c_K\}$ converge to a set of well-separated, linearly independent vectors.
 1032 Geometrically, these prototypes span a support subspace $\mathcal{S}_{code} \subset \mathbb{R}^D$ with an effective rank of
 1033 approximately K .

1034 By minimizing the commitment loss \mathcal{L}_{IVQ} , the optimization process acts as a force pulling the rows
 1035 of Z_p towards these diverse prototypes. Assuming the input image contains diverse visual elements
 1036 that activate a subset of these distinct prototypes, the feature matrix Z_p is effectively regularized to
 1037 span the same subspace as the active codebook vectors:

$$1039 Z_p \xrightarrow{\mathcal{L}_{IVQ}} \text{span}(\{c_k\}_{\text{active}}) \subseteq \mathcal{S}_{code}. \quad (12)$$

1040 Since the codebook maintains full rank ($\approx K$), it acts as a set of semantic anchors that prop open the
 1041 feature space. This imposes an *implicit lower bound* on the feature rank, ensuring that representations
 1042 maintain sufficient dimensionality to encode diverse semantic concepts rather than collapsing
 1043 onto a single manifold.

1044 **3. Structured vs. Indiscriminate Diversity.** This analysis also clarifies why IVQ outperforms
 1045 general-purpose regularization methods like Barlow Twins or Spectral Regularization (as shown in
 1046 Fig. 6).

- 1047 • **General Regularization:** Methods that penalize cross-correlation or maximize spectral
 1048 entropy encourage *indiscriminate diversity*. They force features to be orthogonal regardless
 1049 of semantic content, which can lead to over-regularization where noise or irrelevant textures
 1050 are amplified to satisfy the rank objective.
- 1051 • **IVQ Regularization:** Our method fosters *structured diversity*. It preserves feature rank
 1052 specifically along the semantic directions defined by the clinical concepts (the codebook).
 1053 The feature space is allowed to be low-rank within a concept cluster (compressing intra-
 1054 class variance) while maintaining high-rank separation between different concepts (pre-
 1055 serving inter-class variance). This alignment between optimization dynamics and semantic
 1056 structure is the key driver of IVQ-CBM’s superior performance.

1058 A.4 THEORETICAL ANALYSIS FOR GRADIENT CONVERGENCE

1059 The total loss function $\mathcal{L}_{\text{total}}$ is differentiable with respect to all trainable parameters θ of the
 1060 proposed model. This ensures that gradients are well-defined, permitting stable model training via
 1061 gradient-based optimizers.

1062 *Proof.* The proof proceeds by analyzing the differentiability of each component of the total loss.

1063 **Formal Definitions.** Let $\theta = \{\theta_E, \phi_A, \phi_f, \phi_Q\}$ denote the set of all trainable parameters, where
 1064 θ_E are the parameters of the ViT-based visual encoder \mathcal{E} , ϕ_A are the learnable queries in the Mag-
 1065 net Attention module \mathcal{A} , ϕ_f are the parameters of the projection head f , and ϕ_Q is the learnable
 1066 codebook of the Vector-Quantizer \mathcal{Q} .

1067 The total loss is a weighted sum of its components:

$$1068 \mathcal{L}_{\text{total}}(\theta) = \mathcal{L}_{\text{cls}} + \mathcal{L}_{\text{concept}} + \mathcal{L}_{\text{IVQ}}. \quad (13)$$

1069 By the sum rule of differentiation, if each component loss is differentiable with respect to θ , then
 1070 $\mathcal{L}_{\text{total}}$ is also differentiable. We analyze each component in turn.

1071 **Differentiability of the Main Prediction Path (\mathcal{L}_{cls} and $\mathcal{L}_{\text{concept}}$).** The main prediction path
 1072 computes visual concepts from patch embeddings $\mathbf{Z}_p = \mathcal{E}_{\theta_E}(\mathbf{x}) \in \mathbb{R}^{L \times D}$ and then calculates the clas-
 1073 sification and concept losses. The aggregated visual concepts, denoted $\mathbf{M} \in \mathbb{R}^{K \times D}$, are derived
 1074 as:

$$1075 \mathbf{M} = \mathcal{A}_{\phi_A}(\mathbf{Z}_p), \quad (14)$$

1080 and the final logits are obtained after a projection head f_{ϕ_f} . The Magnet Attention operator \mathcal{A}_{ϕ_A}
 1081 involves computing squared Euclidean distances, applying a ‘softmax’ function, and performing a
 1082 weighted sum via matrix multiplication. The projection head f_{ϕ_f} consists of standard neural network
 1083 layers (e.g., Linear, LayerNorm). All these operations are continuously differentiable.

1084 The losses \mathcal{L}_{cls} and $\mathcal{L}_{\text{concept}}$ are computed using the cross-entropy function, which is smooth and
 1085 differentiable with respect to its inputs. Therefore, by the chain rule, both losses are differentiable
 1086 with respect to the parameters in their computational graphs, namely $\{\theta_E, \phi_A, \phi_f\}$.
 1087

1088 **Differentiability of the VQ Regularization Path (\mathcal{L}_{IVQ})**. This part is critical as the Vector-
 1089 Quantizer \mathcal{Q}_{ϕ_Q} contains a non-differentiable argmin operation for selecting the nearest codebook
 1090 vector $\mathbf{e}_k \in \phi_Q$ for a given input patch feature \mathbf{z}_j :
 1091

$$1092 \quad k^* = \operatorname{argmin}_k \|\mathbf{z}_j - \mathbf{e}_k\|_2^2. \quad (15)$$

1094 The derivative of this discrete selection is zero almost everywhere, which blocks gradient flow. The
 1095 IVQ loss, however, is formulated to circumvent this issue:
 1096

$$1097 \quad \mathcal{L}_{\text{IVQ}} = \underbrace{\|\operatorname{sg}[\mathbf{Z}_p] - \mathcal{Q}_{\phi_Q}(\mathbf{Z}_p)\|_2^2}_{\text{Codebook Loss}} + \beta \cdot \underbrace{\|\mathbf{Z}_p - \operatorname{sg}[\mathcal{Q}_{\phi_Q}(\mathbf{Z}_p)]\|_2^2}_{\text{Commitment Loss}}, \quad (16)$$

1100 where $\operatorname{sg}[\cdot]$ denotes the stop-gradient operator (equivalent to ‘.detach()’).
 1101

1102 We analyze the gradient of each component:

1103

- 1104 • **Gradient w.r.t. codebook ϕ_Q** : The gradient for ϕ_Q flows only through the Codebook Loss
 1105 term, as the Commitment Loss detaches the quantizer’s output. The gradient is:

$$1107 \quad \nabla_{\phi_Q} \mathcal{L}_{\text{IVQ}} = \nabla_{\phi_Q} \|\operatorname{sg}[\mathbf{Z}_p] - \mathcal{Q}_{\phi_Q}(\mathbf{Z}_p)\|_2^2. \quad (17)$$

1108 This gradient is well-defined and updates the codebook vectors to move closer to the en-
 1109 coder’s features.
 1110

- 1111 • **Gradient w.r.t. encoder θ_E** : The gradient for the encoder’s parameters θ_E (which pro-
 1112 duce \mathbf{Z}_p) flows only through the Commitment Loss term. The gradient with respect to the
 1113 encoder’s output is:

$$1115 \quad \nabla_{\mathbf{Z}_p} \mathcal{L}_{\text{IVQ}} = \beta \cdot \nabla_{\mathbf{Z}_p} \|\mathbf{Z}_p - \operatorname{sg}[\mathcal{Q}_{\phi_Q}(\mathbf{Z}_p)]\|_2^2 = 2\beta (\mathbf{Z}_p - \operatorname{sg}[\mathcal{Q}_{\phi_Q}(\mathbf{Z}_p)]). \quad (18)$$

1116 This gradient is well-defined and is equivalent to that of a Mean Squared Error loss. It
 1117 effectively pulls the encoder’s output \mathbf{Z}_p towards the selected (but detached) codebook
 1118 vectors without passing through the non-differentiable argmin operation.
 1119

1120 The use of the stop-gradient operator correctly decouples the updates, ensuring that computable
 1121 gradients are available for both the encoder and the codebook.
 1122

1123 **Conclusion.** We have established the differentiability of all components of the total loss function.
 1124

- 1126 • The prediction losses, \mathcal{L}_{cls} and $\mathcal{L}_{\text{concept}}$, are differentiable with respect to $\{\theta_E, \phi_A, \phi_f\}$.
 1127
- 1128 • The regularization loss, \mathcal{L}_{IVQ} , provides well-defined gradients for both the codebook ϕ_Q
 1129 and the encoder θ_E .
 1130

1131 Since $\mathcal{L}_{\text{total}}$ is a linear combination of these differentiable components, its gradient $\nabla_{\theta} \mathcal{L}_{\text{total}}$ is well-
 1132 defined and can be computed via standard backpropagation. The existence of a valid gradient is a
 1133 necessary condition for the convergence of gradient-based optimization algorithms. Therefore, the
 model architecture is theoretically sound for training. \square

1134 **B IMPLEMENTATION DETAILS**

1135
 1136 **Experimental Setup.** To ensure a fair comparison, we reproduce all baselines within our exper-
 1137 imental framework and adopt Biomedical-CLIP (Zhang et al., 2025) for our method and baselines.
 1138 Based on this architecture, we insert a projection layer to map visual features to the textual feature
 1139 space, thereby aligning their dimensions. We then apply L2 normalization to regularize the aligned
 1140 feature representations. We employ an exponential learning rate scheduler with a warm-up period
 1141 and utilize the AdamW (Loshchilov & Hutter, 2017) optimizer for training. The initial learning rate
 1142 and batch size are set to $1e-4$ and 32, respectively. All experiments are conducted using Python
 1143 3.9, PyTorch 2.5.1, and a single NVIDIA RTX 4090 GPU. We also conduct experiments within
 1144 CLIP to validate the universality of representation collapse (Cherti et al., 2023).

1145 **Concept Generation.** For the concepts associated with each dataset, we prompt Gemini 2.5 Pro to
 1146 generate textual descriptions for each class. The generated concepts are then cross-validated using
 1147 GPT-4o to ensure their quality and relevance. Drawing upon the work of (Panousis et al., 2024), we
 1148 build a hierarchical framework for concepts based on a coarse-to-fine principle.

1150 **C ANALYSIS OF FEATURE RANK DYNAMICS**

1151
 1152 To empirically validate our method’s ability to mitigate **representational collapse**, we analyze the
 1153 dynamics of the feature rank during training. The rank of the feature matrix serves as a proxy for
 1154 the diversity and richness of the learned representations. A sustained high rank indicates that the
 1155 features are diverse and non-redundant, while a decline in rank—known as rank collapse—suggests
 1156 that the feature space has become degenerate, hindering the model’s ability to learn distinct concepts.

1157 In this section, we present a series of experiments comparing our method against various baselines.
 1158 The results consistently demonstrate the effectiveness of our approach in maintaining high-rank
 1159 feature representations.

1160
 1161 **Comparison with State-of-the-Art Baselines.** As illustrated in Figure 4, we first compare our
 1162 model with several leading concept-based methods. Our approach (**Ours**) consistently maintains
 1163 a high and stable feature rank across all eight datasets throughout the training process. In stark
 1164 contrast, baseline methods such as Explicid, MVP-CBM, and others exhibit a noticeable decline in
 1165 feature rank, succumbing to varying degrees of representational collapse. This result highlights our
 1166 method’s superior ability to preserve the expressive power of the feature space compared to existing
 1167 approaches.

1168
 1169 **Comparison on Standard Benchmarks.** As illustrated in Figure 5, we extend our analysis to
 1170 standard vision benchmarks, ranging from CIFAR-10 to large-scale datasets like ImageNet. Con-
 1171 sistent with our observations in the medical domain, our approach (**Ours**) maintains a robust and
 1172 stable feature rank throughout training across all five datasets. In stark contrast, baseline methods
 1173 succumb to varying degrees of representational collapse, a phenomenon that becomes notably more
 1174 severe on complex datasets. Specifically, MVP-CBM and DOT-CBM exhibit a drastic decline in fea-
 1175 ture rank on ImageNet and Places365, indicating a failure to preserve feature diversity at scale. This
 1176 empirical evidence confirms that representational collapse is a fundamental bottleneck in CBMs,
 1177 and highlights our method’s superior ability to generalize and preserve expressive power even in
 1178 large-scale classification scenarios.

1179
 1180 **Ablation Study on the IVQ Module.** To isolate the contribution of our proposed IVQ module,
 1181 we conduct a crucial ablation study, with the results presented in Figure 6. The comparison is
 1182 stark: the model equipped with our IVQ module (w/ IVQ, solid lines) successfully sustains a high
 1183 feature rank on both training and validation sets. Conversely, the model without it (w/o IVQ,
 1184 dashed lines) experiences a sharp drop in rank, mirroring the behavior of the baseline models. This
 1185 provides compelling evidence that the IVQ module is the key component responsible for preventing
 1186 feature space degeneracy and maintaining representational diversity.

1187
 1188 **Comparison with Representation Regularization Techniques.** Furthermore, we extend our
 1189 analysis to include other common representation regularization techniques in Figure 7. While some

regularization methods may also help in maintaining a higher feature rank, it is crucial to note a key insight: **a high feature rank is a necessary, but not sufficient, condition for superior performance.** Simply forcing features to be diverse (e.g., via decorrelation penalties) does not guarantee that they are meaningful or well-aligned with the downstream task. As shown in the figure, our method not only preserves rank effectively but also achieves this in a way that structures the feature space for better concept learning, ultimately leading to improved overall performance (as shown in [section 4.2](#)). This distinguishes our approach from methods that might artificially inflate rank without enhancing semantic representation.

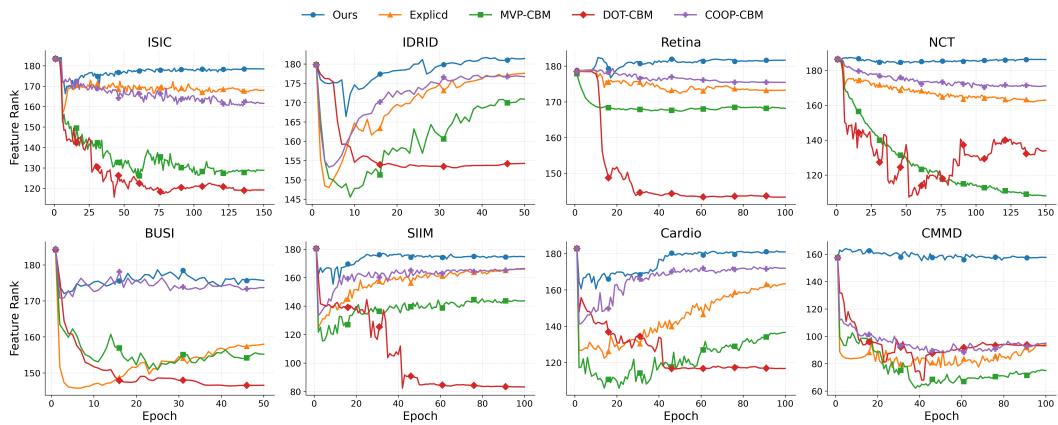


Figure 4: Comparative analysis of feature rank dynamics across eight datasets. Our proposed method (**Ours**) successfully maintains a high and stable feature rank, while baseline methods, including Explicid, MVP-CBM, DOT-CBM, and COOP-CBM, exhibit varying degrees of rank collapse during training.

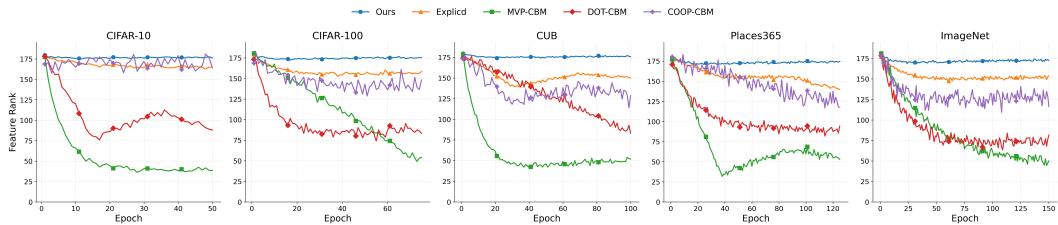


Figure 5: Comparative analysis of feature rank dynamics across five general domain datasets. Our proposed method (**Ours**) successfully maintains a high and stable feature rank, while baseline methods, including Explicid, MVP-CBM, DOT-CBM, and COOP-CBM, exhibit varying degrees of rank collapse during training.

D VISUALIZATION OF CODEBOOK IN IVQ

To qualitatively evaluate the semantic knowledge captured by the IVQ codebook, we provide a comprehensive visual analysis across all six medical imaging datasets. In the following figures, we visualize the prototype index maps for representative images. For each image patch, we identify the nearest codebook prototype via an argmin operation and color-code the patch according to that prototype’s index. This process generates a concept activation heatmap, revealing which learned visual prototype is most dominant in each region of the image. The results consistently demonstrate that our model learns semantically meaningful and clinically relevant concept representations that align with the diagnostic reasoning of medical experts.

Analysis on CMMD (Mammography). As shown in [Figure 8a](#), the resulting mapping demonstrates a highly logical process that mirrors clinical reasoning. The prototype for Mass Margin precisely delineates the lesion’s contour, while those for Mass Shape and Calcification Features correspond to its internal characteristics. Crucially, the prototype for Associated Features extends its focus beyond the lesion’s border, probing the surrounding parenchyma for signs of structural distortion—a key indicator of malignancy.

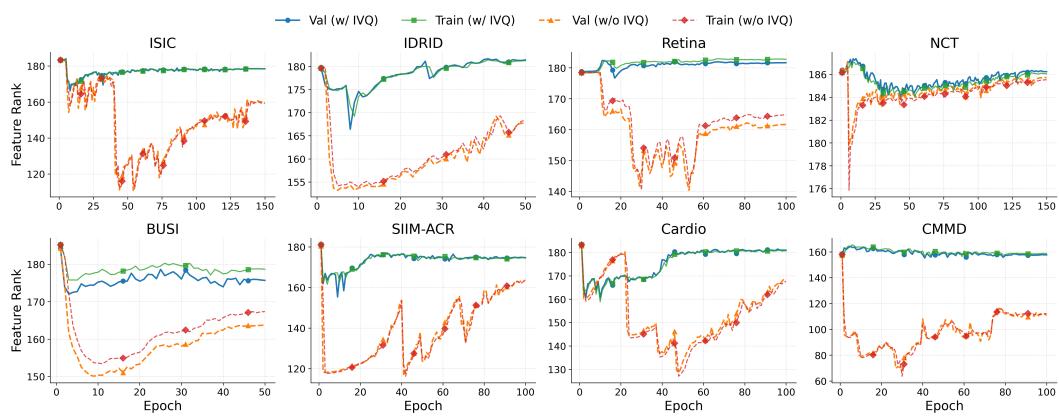


Figure 6: Feature rank dynamics for models with (w/ IVQ, solid lines) and without (w/o IVQ, dashed lines) our IVQ module, shown on both training and validation sets. The clear gap demonstrates the effectiveness of IVQ in preventing rank collapse.

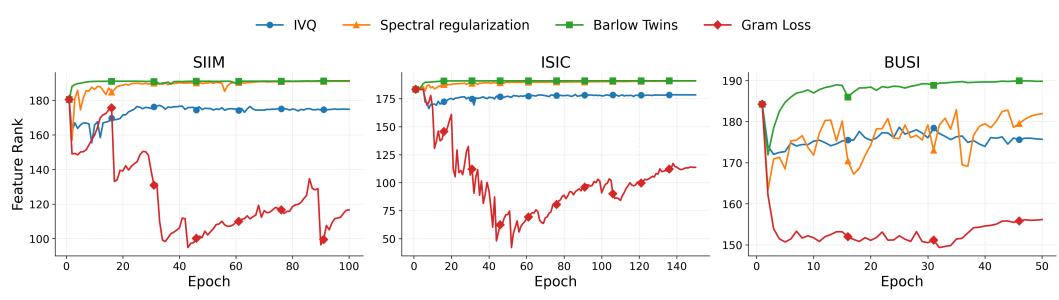


Figure 7: Feature rank dynamics of IVQ against regularization baselines on the SIIM, ISIC, and BUSI datasets. IVQ (blue) and Barlow Twins (green) successfully maintain a high rank, while Spectral regularization (orange) is unstable and Gram Loss (red) suffers a severe collapse.

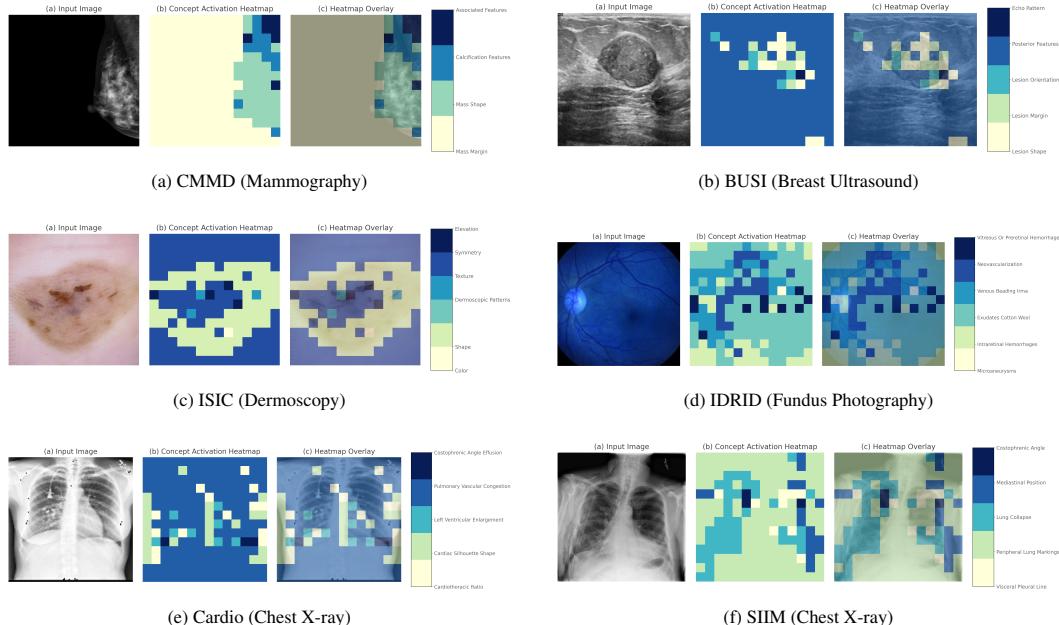


Figure 8: Visualization of the learned codebook prototype mappings across six medical imaging datasets. For each dataset, we show (a) the input image, (b) the concept activation heatmap where each color corresponds to the most active prototype for that patch, and (c) the overlay. The color legend maps each prototype to a human-defined clinical concept.

1296 **Analysis on BUSI (Breast Ultrasound).** The visualization for BUSI in [Figure 8b](#) reveals a structured
 1297 analysis of the breast lesion. The prototypes for **Lesion Shape** and **Lesion Margin**
 1298 accurately capture the overall form and boundary of the hypoechoic mass. Progressing to finer de-
 1299 tails, the prototypes for **Posterior Features** and **Echo Pattern** are activated on the internal
 1300 and posterior regions of the lesion, which are critical assessments in the BI-RADS classification
 1301 system.

1302 **Analysis on ISIC (Dermoscopy).** In the dermoscopy example [Figure 8c](#), the prototype mappings
 1303 align well with clinical assessment criteria like the "ABCDE" rule. Prototypes for general attributes
 1304 such as **Shape** and **Color** are active across the broader lesion area. Meanwhile, more specific
 1305 and clinically crucial prototypes, like **Dermoscopic Patterns** and **Texture**, are correctly
 1306 localized to the darker, diagnostically significant interior regions.

1307 Most importantly, this visualization addresses the critical issue of concept ambiguity ([Kim et al., 2023](#)), where a given image may lack a specific concept entirely—a key challenge for concept-
 1308 based models. For instance, while this lesion has a distinct texture, it may not exhibit **Streaks**.
 1309 Our model correctly reflects this by showing negligible activation for the corresponding prototype.
 1310 This demonstrates a faithful alignment, as the model does not erroneously force a prediction for a
 1311 feature that is not visually present, confirming that our learned codebook achieves a truly accurate
 1312 and discerning concept assignment.

1313 **Analysis on IDRID (Fundus Photography).** The analysis of the diabetic retinopathy case in [Figure 8d](#)
 1314 shows that the model differentiates between various pathologies. While general findings
 1315 like **Intraretinal Hemorrhages** are mapped to wider areas, the prototypes for severe, high-
 1316 risk pathologies such as **Neovascularization** and **Vitreous Hemorrhage** are correctly
 1317 concentrated near critical anatomical structures like the optic disc and major vascular arcades.

1318 **Analysis on Cardio & SIIM (Chest X-ray).** The chest X-ray visualizations [Figure 8e](#) and
 1319 [Figure 8f](#) demonstrate a strong anatomical grounding. Prototypes for global assessments like
 1320 **Cardiothoracic Ratio** and **Cardiac Silhouette Shape** are broadly active over the
 1321 heart. In contrast, prototypes for specific pathologies are precisely localized. For instance,
 1322 **Pulmonary Vascular Congestion** is mapped to the lung fields, while **Costophrenic**
 1323 **Angle Effusion** is correctly activated in the lower lobes of the lungs where pleural fluid
 1324 accumulates. This showcases a spatially aware reasoning process that distinguishes between global
 1325 shape and localized pathological signs.

1326 **Codebook Visualization Reveals Structured and Disentangled Concepts.** To qualitatively as-
 1327 sess the structure of the learned codebook, we visualize the code vectors using UMAP by projecting
 1328 them into a 3D space. As illustrated in [Figure 9](#), a clear and consistent pattern emerges across all six
 1329 distinct datasets. The learned codes for each dataset are well-separated, forming discrete and com-
 1330 pact clusters with significant distance between them. This spatial separation is highly desirable, as
 1331 it indicates that the learned codes are disentangled and non-redundant. Each code has successfully
 1332 converged to represent a unique, semantically distinct concept, avoiding representational collapse
 1333 where multiple codes might capture similar features. The consistency of this structured outcome
 1334 across diverse medical imaging modalities—from ultrasound (BUSI) and mammography (CMM)
 1335 to dermoscopy (ISIC) and beyond—demonstrates the robustness and generalizability of our method
 1336 in discovering a meaningful basis of concepts. The formation of such a clean and well-structured
 1337 codebook is foundational to the model’s ability to make interpretable and reliable predictions.

1343 E VISUALIZATION OF CODEBOOK IN VQ

1344 For comparison, we visualize the prototype mappings learned by a standard VQ baseline in [Figure 10](#). This ablation study qualitatively demonstrates the limitations of standard VQ, which
 1345 struggles to learn semantically meaningful and spatially-precise concepts. In stark contrast to the
 1346 clinically-aligned prototypes from our proposed IVQ method, the VQ baseline’s mappings often re-
 1347 veal a significant lack of anatomical grounding. The resulting heatmaps show concepts activated in

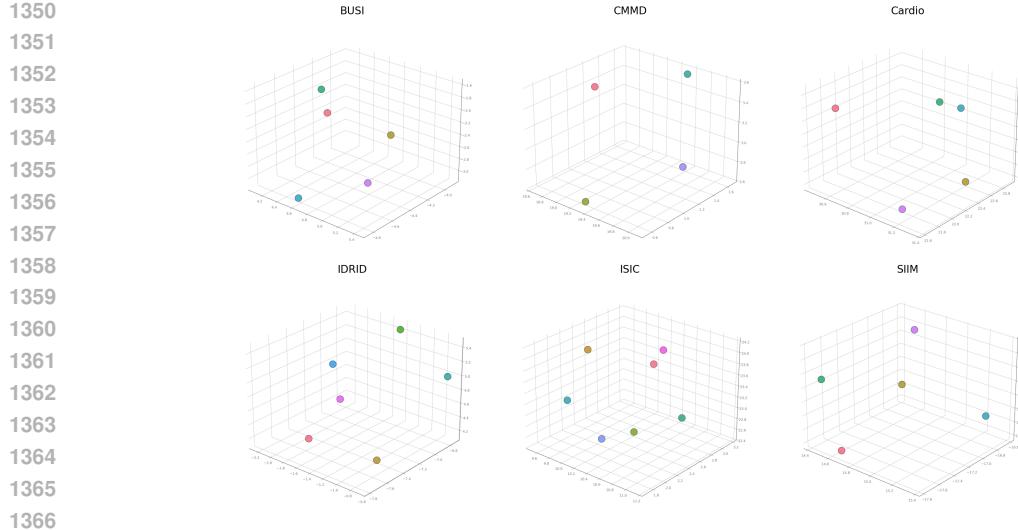


Figure 9: UMAP visualization for the codebook in various datasets. The clear spatial separation between codes in each plot indicates a highly disentangled and non-redundant set of learned concepts. This consistent structure across all domains demonstrates the robustness of our method in discovering a meaningful conceptual basis.

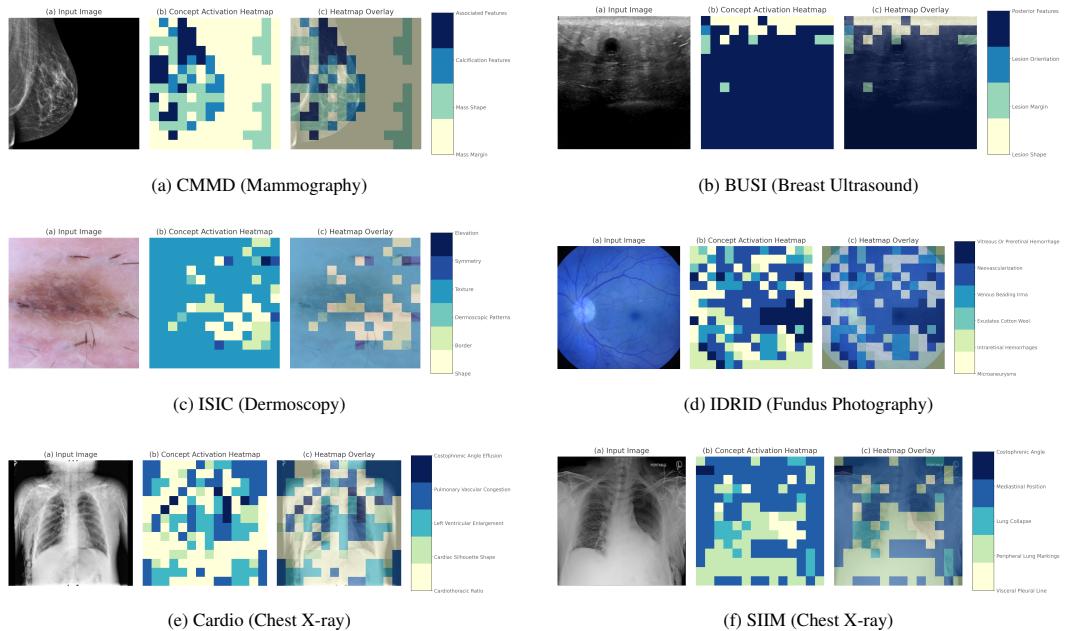


Figure 10: Visualization of the learned codebook prototype mappings from the standard VQ baseline. These mappings highlight a significant failure in capturing clinically-relevant concepts. Prototypes are often scattered, misaligned with anatomical structures, and fail to differentiate between pathology and background, starkly contrasting with the precise mappings of our IVQ model (shown in Figure 8).

nonsensical locations, failing to distinguish between critical pathologies and irrelevant background, thus highlighting the necessity of our IVQ approach.

Analysis on CMMMD (Mammography). The VQ mapping in Figure 10a fails to capture any meaningful anatomical structure. The prototype for Mass Margin (yellow) is nonsensically activated in the background adipose tissue rather than on the lesion's contour. Similarly, Mass Shape (light green) and Calcification Features (blue) are scattered randomly, failing to delineate the

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actual lesion or its internal characteristics. This mapping lacks the logical, clinically-relevant precision required for diagnosis.

Analysis on BUSI (Breast Ultrasound). The BUSI visualization (Figure 10b) demonstrates a near-total failure of the VQ model. The actual hypoechoic lesion is almost entirely ignored or misclassified as the Posterior Features (dark blue) prototype, which dominates the entire image background. Critical concepts like Lesion Shape and Lesion Margin are only sparsely and incorrectly activated in the surrounding tissue, showing no understanding of the target pathology.

Analysis on ISIC (Dermoscopy). This mapping (Figure 10c) shows poor conceptual differentiation. The prototype for Dermoscopic Patterns (light green) incorrectly dominates almost the entire image, including the clear background skin, indicating it has not learned a specific feature. Furthermore, Border and Shape prototypes are activated illogically inside the lesion rather than at its periphery, reversing the correct diagnostic process.

Analysis on IDRID (Fundus Photography). The VQ mapping for IDRID (Figure 10d) is chaotic and lacks anatomical precision. High-risk pathologies like Neovascularization and Venous Beading are scattered randomly across the retina, failing to co-localize with critical structures like the optic disc or major vascular arcades. This all-over-the-place activation suggests the model has only learned coarse pixel statistics rather than a true, spatially-aware understanding of the pathology.

Analysis on Cardio & SIIM (Chest X-ray). The chest X-ray visualizations demonstrate severe anatomical flaws. In the Cardio example (Figure 10e), the prototype for Cardiotoracic Ratio (yellow) bleeds nonsensically into the lung fields and abdomen. Critically, Costophrenic Angle Effusion (dark blue) is activated in the *upper* lung zones, which is clinically impossible as fluid accumulates at the lung bases. Similarly, in the SIIM image (Figure 10f), the Costophrenic Angle (dark blue) is again misplaced in the upper chest, and the Visceral Pleural Line prototype fails to trace the actual line of the collapsed lung.

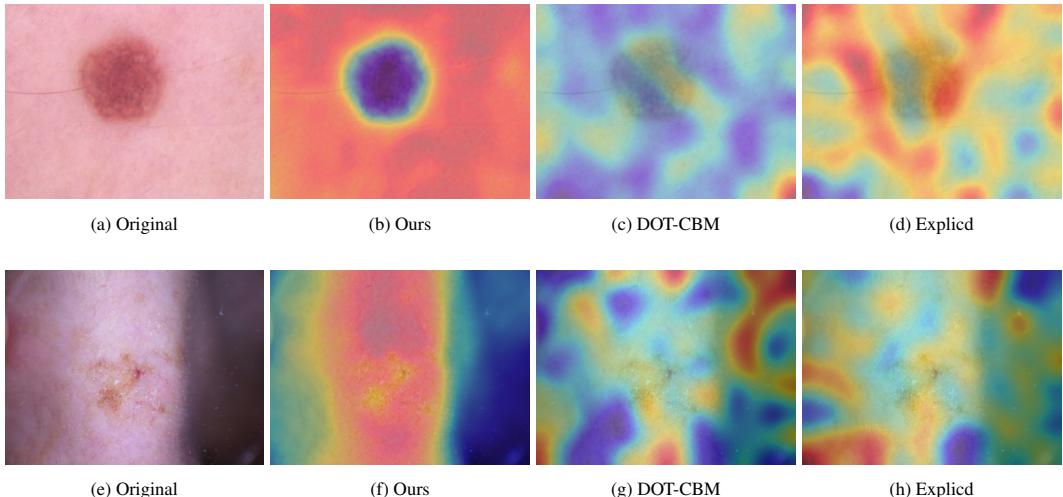


Figure 11: **Qualitative comparison of explanation heatmaps on ISIC 2018 dermoscopy images (skin lesion classification).** We visualize concept attributions using Grad-CAM-style activation maps (Selvaraju et al., 2019) applied to the concept bottleneck layer (or post-hoc concept predictor) of each method, overlaid on the original images with jet colormap and 40% opacity. Our method consistently produces sharp, highly localized activations that precisely delineate clinically relevant lesion regions while effectively suppressing background skin and artifacts. In contrast, DOT-CBM and ExpIcld generate diffuse, noisy, or poorly localized patterns that frequently spill into surrounding healthy skin or fail to adequately highlight diagnostic features of the lesion.

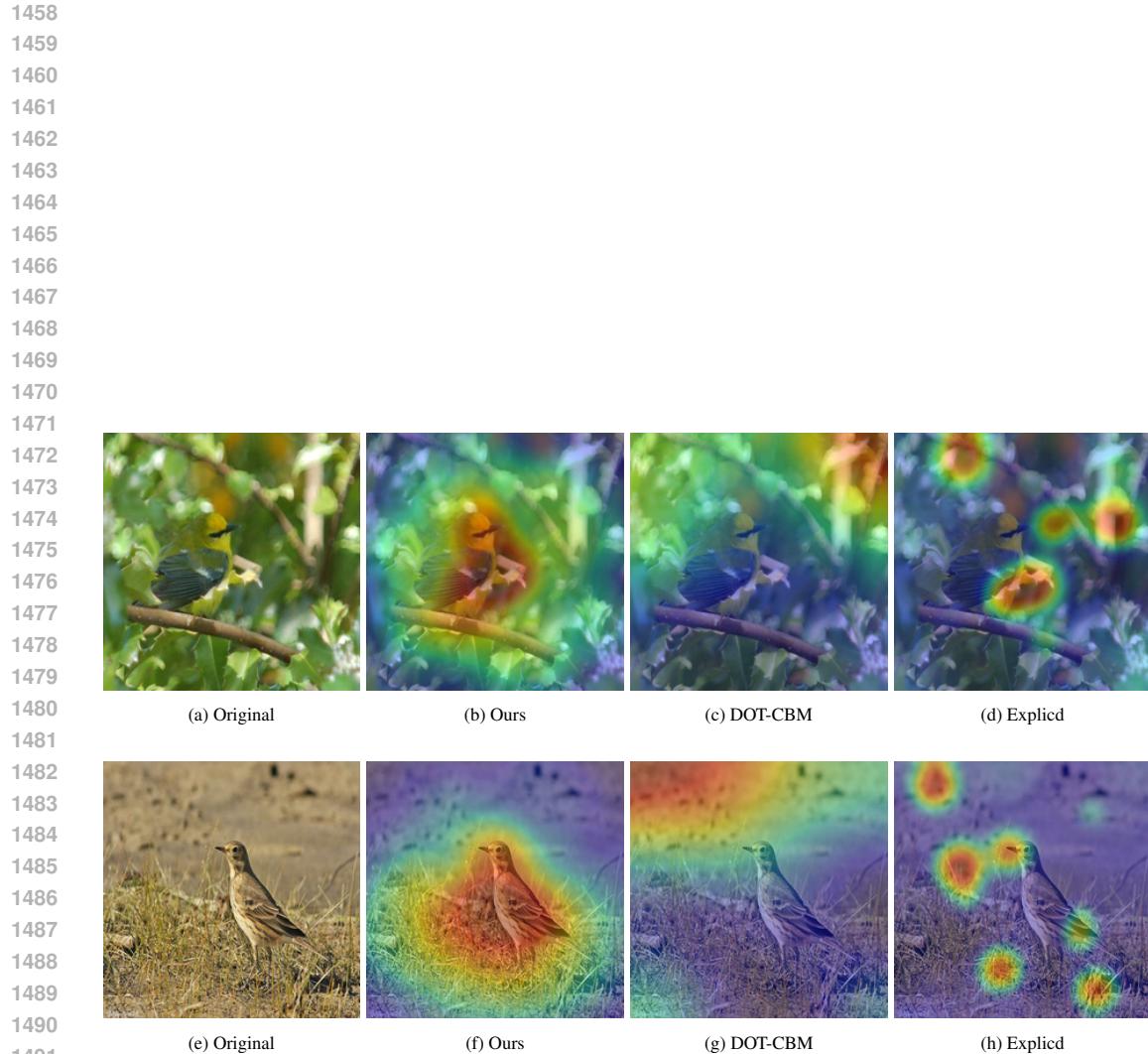


Figure 12: **Qualitative comparison of explanation heatmaps on the CUB-200-2011 dataset (fine-grained bird classification).** We visualize concept attributions using Grad-CAM-style activation maps (Selvaraju et al., 2019) applied to the concept bottleneck layer (or post-hoc concept predictor) of each method, overlaid on the original images with jet colormap and 40% opacity. Our approach consistently generates sharp, well-localized activations that faithfully highlight the entire discriminative bird regions (head, breast, wings, and tail) while effectively suppressing irrelevant background. By contrast, DOT-CBM and Explicd produce diffuse, over-smoothed, or noisy activation patterns that either leak into background areas or fail to adequately cover diagnostically relevant bird parts.

1512 F VISUALIZATION ANALYSIS WITH BASELINES

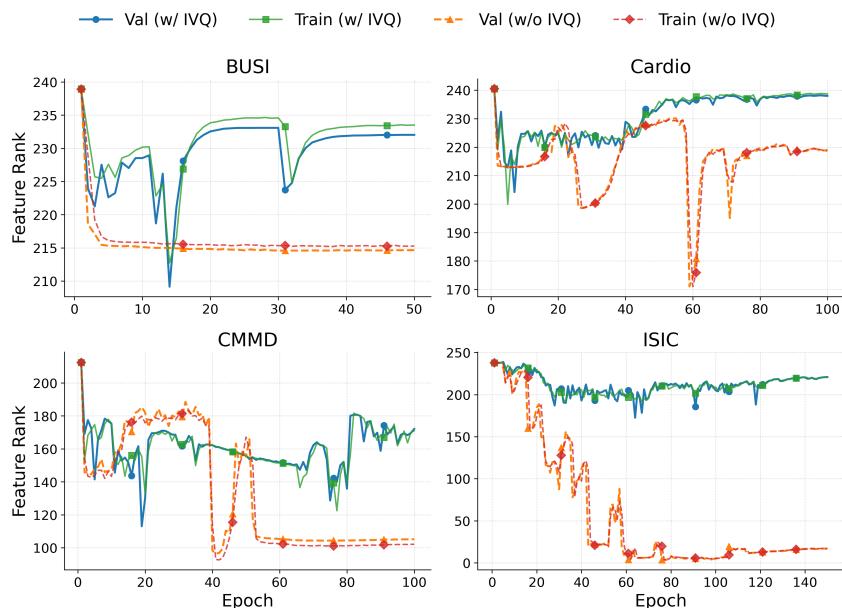
1514 To empirically evaluate the faithfulness and localization quality of the learned concepts, we conduct
 1515 a qualitative comparison between our proposed IVQ-CBM and two recent patch-based baselines:
 1516 DOT-CBM and Explicd. We employ Grad-CAM (Selvaraju et al., 2019) to generate concept activa-
 1517 tion maps, visualizing the spatial regions that contribute most significantly to the model’s concept
 1518 predictions. This analysis is performed across two distinct domains: medical imaging (ISIC 2018)
 1519 and fine-grained object classification (CUB-200-2011).

1520 **Medical Imaging (ISIC 2018).** Figure 11 presents the visualization results on dermoscopy im-
 1521 ages. The comparison reveals a stark contrast in the semantic coherence of the learned features.
 1522 Our method (Columns (b) and (f)) produces sharp, object-centric activations that precisely delineate
 1523 the lesion boundaries, effectively separating the pathological tissue from healthy skin. In contrast,
 1524 the baselines exhibit severe visual degradation indicative of representational collapse. DOT-CBM
 1525 (Columns (c) and (g)) displays diffuse, “cloudy” activation patterns that spill significantly into the
 1526 background, suggesting a failure to disentangle foreground concepts from noise. Similarly, Explicd
 1527 (Columns (d) and (h)) suffers from scattered and disjointed activations that often miss the lesion
 1528 center entirely. These visual artifacts confirm that without explicit regularization to maintain feature
 1529 rank, the resulting concept representations become informationally redundant and spatially ambigu-
 1530 ous.

1531 **General Object Classification (CUB-200-2011).** To demonstrate generalizability, we extend this
 1532 analysis to the CUB-200-2011 dataset in Figure 12. Consistent with the medical domain, our ap-
 1533 proach generates well-localized heatmaps that cover discriminative avian parts (e.g., head, wings,
 1534 torso) while suppressing complex background clutter. Conversely, the baselines struggle with lo-
 1535 calization; their activations are either over-smoothed or erroneously highlight background elements
 1536 (e.g., branches or ground).

1537 **Conclusion.** The superior visualization quality of IVQ-CBM—characterized by precise localization
 1538 and boundary adherence—is not merely a result of better training dynamics but a direct phenomeno-
 1539 logical manifestation of our high-rank feature space. By successfully escaping the low-rank trap via
 1540 Implicit Vector Quantization, our model preserves the semantic diversity required for faithful and
 1541 interpretable visual concept learning.

1542 G RESULTS WITH OTHER MULTI-MODAL BACKBONE



1564 **Figure 13:** Ablation study on the impact of the IVQ component. The figure compares the feature rank dynam-
 1565 ics of the model trained with and without the IVQ module with CLIP backbone, demonstrating its effect on
 representation diversity.

1566 Our primary experiments are conducted on a CLIP model pre-trained with a biomedical corpus
 1567 (Zhang et al., 2025) to build the proposed IVQ-CBM. This domain-specific backbone ensures
 1568 feature relevance for medical tasks. Within this main setup, we perform comprehensive ablation
 1569 studies to validate the contribution of each component. Figure 6 provides a compelling visualization
 1570 of a crucial ablation study on the IVQ module. The results are unequivocal: the model variant with-
 1571 out IVQ (dashed lines) suffers a significant drop in feature rank during training, a clear indication of
 1572 representational collapse. In stark contrast, the full model equipped with IVQ (solid lines) robustly
 1573 maintains a high feature rank throughout the training process. Notably, on datasets such as BUSI
 1574 and CMMD, it even exhibits rank recovery after initial dips. This direct comparison underscores the
 1575 indispensable role of IVQ in preserving feature space dimensionality and preventing catastrophic
 1576 rank collapse.

1577 A key question is whether the observed rank collapse is specific to the domain-adapted biomedical
 1578 encoder or if it represents a more general challenge in representation learning. To investigate this,
 1579 we replicated the experiment using a general-purpose feature extractor. Specifically, we replaced
 1580 the specialized backbone with a standard pre-trained Vision Transformer (ViT-L/14) (Radford et al.,
 1581 2021), with weights from the OpenCLIP project (Cherti et al., 2023) trained on the LAION-2B
 1582 dataset (Schuhmann et al., 2022). As demonstrated in Figure 13, the results on four distinct datasets
 1583 are unequivocal. The models trained without our IVQ module (dashed lines) consistently suffer
 1584 from a severe drop in feature rank, confirming that representational collapse is not tied to a specific
 1585 encoder. In stark contrast, the models equipped with IVQ (solid lines) robustly maintain a high and
 1586 stable feature rank throughout training. This confirms that rank collapse is a fundamental problem
 1587 and establishes IVQ as a robust, model-agnostic solution for preserving representation diversity.

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H STATEMENT ON THE USE OF LARGE LANGUAGE MODELS

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1612 Throughout the preparation of this manuscript, we utilized large language models to enhance the
 1613 quality of the text. Specifically, we employed Google’s Gemini Pro for tasks related to language
 1614 refinement, including correcting grammar and spelling, improving sentence clarity, and ensuring a
 1615 consistent academic tone.

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1619 The core scientific contributions, including the formulation of the problem, the proposed methodol-
 1616 ogy, the design and execution of experiments, and the interpretation of results, are entirely the work
 1617 of the authors. All text generated or modified by the LLM was meticulously reviewed, edited, and
 1618 revised by the authors to ensure it accurately reflects our original ideas and findings. The authors
 1619 bear full and final responsibility for all content presented in this paper.

1620 **I PSEUDOCODE OF IVQ-CBM**
16211622 **Algorithm 1** Training Procedure of Our Proposed Method

1623 **Require:** Training dataset $\mathcal{D} = \{(x, \mathbf{c}, y)\}$.
 1624 **Require:** Visual encoder E_I , text encoder E_t , classifier head h_{cls} .
 1625 **Require:** Learnable concept queries $\mathbf{Q} \in \mathbb{R}^{K \times D}$.
 1626 **Require:** Learnable IVQ codebook $\mathcal{C}_{vq} \in \mathbb{R}^{K \times D}$.
 1627 **Require:** Commitment cost hyperparameter β .
 1628 **Require:** Set of textual concept descriptions $\{t_k\}_{k=1}^K$.
 1629
 1630 1: Initialize parameters for E_I , h_{cls} , \mathbf{Q} , and \mathcal{C}_{vq} .
 1631 2: Pre-compute text concept embeddings: $\tau_k \leftarrow E_t(t_k)$ for $k = 1, \dots, K$.
 1632 3: **for** each training epoch **do**
 1633 4: **for** each batch (x, \mathbf{c}, y) sampled from \mathcal{D} **do** ▷ 1. Visual Feature Extraction
 1634 5: 6: $\mathbf{Z}_v = [\mathbf{z}_{cls}, \mathbf{z}_1, \dots, \mathbf{z}_L] \leftarrow E_I(x)$ ▷ Encode image
 1635 7: $\mathbf{Z}_p \leftarrow [\mathbf{z}_1, \dots, \mathbf{z}_L]$ ▷ Extract patch-level features
 1636 8: 9: Compute soft-assignment matrix $\mathbf{A} \in \mathbb{R}^{L \times K}$ between patches and queries: ▷ 2. Magnet Concept Aggregation
 1637 10: $A_{jk} \leftarrow \frac{\exp(-\|\mathbf{z}_j - \mathbf{q}_k\|_2^2)}{\sum_{k'=1}^K \exp(-\|\mathbf{z}_j - \mathbf{q}_{k'}\|_2^2)}$ ▷ For each patch j and query k
 1638 11: $\mathcal{M} \leftarrow \mathbf{A}^\top \mathbf{Z}_p$ ▷ Aggregate features into K Visual Concepts
 1639 12: 13: $\mathbf{v} \leftarrow \text{diag}(\mathcal{M} \tau^\top)$ ▷ 3. Concept-Text Alignment
 1640 14: 15: $\mathbf{p} \leftarrow h_{cls}(\mathbf{v})$ ▷ Generate Concept Activation Vector (CAV)
 1641 16: 17: $\mathcal{L}_{cls} \leftarrow \mathcal{L}_{CE}(\mathbf{p}, y)$ ▷ 4. Final Classification
 1642 18: $\mathcal{L}_{concept} \leftarrow \mathcal{L}_{BCE}(\mathbf{v}, \mathbf{c})$ ▷ Predict class logits from CAV
 1643 19: ▷ – Implicit Vector Quantization (IVQ) Regularization –
 1644 20: For each patch feature $\mathbf{z}_j \in \mathbf{Z}_p$, find nearest codebook vector $\mathbf{c}_{k_j} \in \mathcal{C}_{vq}$.
 1645 21: Let $\mathbf{Z}_q = [\mathbf{c}_{k_1}, \dots, \mathbf{c}_{k_L}]$ be the matrix of quantized features.
 1646 22: $\mathcal{L}_{IVQ} \leftarrow \|\text{sg}(\mathbf{Z}_p) - \mathbf{Z}_q\|_2^2 + \beta \|\mathbf{Z}_p - \text{sg}(\mathbf{Z}_q)\|_2^2$ ▷ IVQ loss
 1647 23: ▷ – Overall Objective and Optimization –
 1648 24: $\mathcal{L} \leftarrow \mathcal{L}_{cls} + \mathcal{L}_{concept} + \mathcal{L}_{IVQ}$ ▷ Total loss
 1649 25: Update parameters of $E_I, h_{cls}, \mathbf{Q}, \mathcal{C}_{vq}$ using gradients from \mathcal{L} .
 1650 26: **end for**
 1651 27: **end for**

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 1659 **J QUANTITATIVE INTERPRETABILITY AND CAUSAL FAITHFULNESS**
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1661 While qualitative visualizations offer intuitive insights, rigorous validation requires quantifying how
 1662 well the learned concepts align with human expertise and whether they causally drive the model’s
 1663 decisions. To this end, we conducted two supplementary studies: a human evaluation with radiolo-
 1664 gists and a concept intervention test.

1666 **J.1 HUMAN EVALUATION WITH EXPERT RADIOLOGISTS**
1667

1668 To assess the spatial and semantic alignment of our learned codebook prototypes with clinical knowl-
 1669 edge, we invited two radiologists to participate in a blinded evaluation study.

1670 **Experimental Protocol.** We randomly sampled 50 images across four diverse datasets: CMMD
 1671 (mammography), BUSI (ultrasound), ISIC (dermoscopy), and IDRID (fundus photography). The
 1672 evaluation comprised two distinct tasks:

1674

1675 1. **Concept Localization (Spatial):** Experts were presented with an image and a target clin-
1676 ical concept (e.g., *Mass Margin*). They rated the model-generated activation heatmap on a
1677 5-point Likert scale (1 = Completely Misaligned, 5 = Perfectly Aligned) based on whether
1678 the highlighted region corresponded to the clinical pathology.

1679 2. **Semantic Alignment (Conceptual):** Experts viewed the image and the heatmap *without*
1680 the concept label. They were asked to identify the represented concept from a multiple-
1681 choice list containing the ground truth and 3–4 plausible semantic distractors (e.g., distin-
1682 guishing *Calcification* from *Mass Margin*).

1683

1684 **Table 6: Quantitative Human Evaluation Results.** Two radiologists evaluated the interpretability of IVQ-
1685 CBM on localization quality (Likert Scale 1–5) and semantic consistency (Choice Accuracy).

Dataset	Task 1: Localization Accuracy (Avg. Likert Score, 1–5)	Task 2: Semantic Alignment (Avg. Choice Accuracy)
CMMD (Mammography)	4.32	90% (45/50)
BUSI (Ultrasound)	4.51	92% (46/50)
ISIC (Dermoscopy)	4.15	88% (44/50)
IDRID (Fundus Photography)	4.20	86% (43/50)
Average	4.30	89%

1693 **Results.** As detailed in Table 6, IVQ-CBM achieved a high average localization score of **4.30/5.0**
1694 and a semantic alignment accuracy of **89%**. These results quantitatively corroborate that our IVQ
1695 mechanism successfully anchors visual features to semantically meaningful and spatially accurate
1696 clinical concepts.

1697 **Table 7: Concept Intervention Test on CMMD.** We measure the drop in the model’s predicted probability for
1698 the “Malignant” class after manually intervening on specific concept activations. The substantial drop confirms
1699 the causal role of these concepts in the decision process.

Intervention Type	Avg. $P(\text{Malignant})$	Relative Change
None (Baseline)	0.96	–
Intervene on “Mass Margin”	0.80	-16.7%
Intervene on “Mass Shape”	0.85	-11.5%
Intervene on Both	0.72	-25.0%

1710 J.2 CAUSAL FAITHFULNESS VIA CONCEPT INTERVENTION

1711 A critical requirement for CBMs is *causal faithfulness*—meaning the concepts should not merely
1712 correlate with the prediction but actively drive it. We validated this via a counterfactual intervention
1713 test on the CMMD dataset.

1714 **Methodology.** We selected a test subset of 50 images where the model confidently predicted malign-
1715 ancy ($P(\text{Malignant}) > 0.9$). We identified clinically causal concepts for this decision, specifically
1716 *Spiculated Margin* and *Irregular Shape*. We then performed an intervention on the Concept Acti-
1717 vation Vector (CAV), denoted as v . Specifically, we “flipped” the activation scores of these malignant
1718 concepts by replacing them with the average scores derived from benign samples, while keeping
1719 the classification head h_{cls} frozen. We then measured the degradation in the model’s predicted
1720 probability for the malignant class.

1721 **Results.** Table 7 demonstrates the impact of these interventions. Modifying individual concepts re-
1722 sulted in a notable decrease in confidence. Crucially, intervening on both shape and margin concepts
1723 caused a substantial **25.0% drop** in the predicted probability (from 0.96 to 0.72). This significant
1724 sensitivity confirms that the decision-making logic of IVQ-CBM causally relies on these high-level
1725 clinical concepts, rather than spurious correlations or background artifacts.

1728 **K ANALYSIS OF INFORMATION LEAKAGE AND EFFECTIVE CONCEPT**
 1729 **LEARNING**

1731 Recent studies (Yan et al., 2023; Srivastava et al., 2025) have highlighted a critical challenge in
 1732 CBM: the potential for information leakage in the bottleneck layer, where models may achieve high
 1733 accuracy by encoding non-semantic noise rather than learning meaningful concepts. To rigorously
 1734 validate the faithfulness of our approach, we evaluate IVQ-CBM using the A-NEC (Accuracy at
 1735 Number of Effective Concepts) metric proposed by Srivastava et al. (2025) and provide a theoretical
 1736 analysis of the mechanisms inherent to our architecture that mitigate such leakage.

1738 **K.1 ROBUSTNESS EVALUATION ON THE A-NEC METRIC**

1740 The A-NEC metric assesses whether a model relies on a concise set of “effective” concepts or
 1741 exploits a diffuse sum of features (leakage). We conducted an evaluation on both natural (CUB,
 1742 CIFAR-10) and medical (ISIC, BUSI) datasets. Specifically, we performed post-hoc pruning on
 1743 the final classification layer, retaining only the top-5 contributing concepts for each class prediction
 1744 (denoted as ANEC-5), and compared this restricted performance against that of the full model.

1745 Table 8: Evaluation of IVQ-CBM on the ANEC-5 Metric. The results demonstrate minimal performance
 1746 degradation when restricting the model to the top-5 effective concepts, indicating robustness against informa-
 1747 tion leakage.

Dataset	Domain	Full Model Acc (%)	ANEC-5 Acc (%)	Performance Drop (Δ)
CUB	Natural	75.93	75.21	-0.72%
CIFAR-10	Natural	87.92	86.85	-1.07%
ISIC	Medical	90.11	89.20	-0.91%
BUSI	Medical	93.59	92.80	-0.79%

1755 As presented in Table 8, IVQ-CBM retains over 98% of its original performance across all datasets
 1756 even when restricted to utilizing only the top-5 concepts. This minimal performance drop indicates
 1757 that the model’s decision-making is primarily driven by a few highly relevant semantic concepts,
 1758 rather than relying on residual leakage distributed across irrelevant dimensions.

1761 **K.2 MECHANISM ANALYSIS: MITIGATING LEAKAGE VIA STRUCTURAL REGULARIZATION**

1763 While prior approaches mitigate leakage by enforcing sparsity constraints on classifier weights,
 1764 IVQ-CBM addresses the root cause—feature representation—through two complementary mecha-
 1765 nisms:

1768 **IVQ as a Semantic Filter.** Information leakage often exploits high-frequency noise or low-rank
 1769 degenerate subspaces that carry discriminative but non-semantic information. The proposed IVQ
 1770 mechanism acts as a structure-inducing regularizer. By imposing the Commitment Loss (Eq. 4),
 1771 continuous patch features are compelled to align with learned codebook prototypes, which function
 1772 as semantic anchors. This process effectively filters out unstructured noise, as leakage patterns
 1773 typically lack the statistical consistency to form stable clusters within the codebook. By enforcing
 1774 semantic consistency with discrete prototypes, IVQ prevents the bottleneck from serving as a generic
 1775 conduit for pixel-level noise.

1778 **Magnet Attention as Implicit Sparsity.** The Magnet Attention mechanism aggregates features
 1779 via a competitive Softmax dynamic. This introduces an *implicit sparsity* effect: patches must “vote”
 1780 strongly for specific concept queries to be aggregated. Diffuse background noise or leakage, which
 1781 typically manifests as weak, uniform signals across patches, is naturally suppressed by the exponential
 1782 nature of the Softmax function. Consequently, the resulting Visual Concepts \mathcal{M} are composed

1782 of strong, concept-aligned signals, effectively achieving the goal of effective concept learning during
 1783 the feature aggregation stage.

1786 K.3 IVQ CODEBOOK AS A DIAGNOSTIC TOOL FOR CONCEPT REFINEMENT

1788 Beyond its role as a regularizer, the IVQ codebook offers a unique capability: it functions as a trans-
 1789 parent diagnostic tool to audit the quality of predefined textual concepts. Since the commitment loss
 1790 (Eq. 4) compels codebook vectors to serve as semantic anchors for visual patches, we hypothesize
 1791 that the frequency of patch assignments to each prototype serves as a quantitative proxy for that
 1792 concept’s visual validity.

1793 To validate this, we conducted a post-hoc analysis of prototype assignment statistics on the ISIC
 1794 dataset. The analysis revealed a stark dichotomy: while robust concepts such as *Blue-whitish veil*
 1795 attracted tens of thousands of patch assignments, the concept *Rough Texture* received negligible
 1796 attention (< 50 assignments across the entire validation set). This quantitative signal suggests that
 1797 *Rough Texture* is a tactile property ill-suited for 2D dermoscopy classification, effectively rendering
 1798 it a null concept in the visual domain.

1799 Leveraging this insight, we implemented a closed-loop refinement process summarized in Table 9.
 1800 We replaced the ineffective concept with a more visually distinct alternative, *Irregular Streaks*, and
 1801 retrained the model. As shown in the table, this targeted adjustment yielded a tangible performance
 1802 improvement, boosting Accuracy to **90.75%** (+0.64%) and BMAC to **87.12%** (+0.90%). This ex-
 1803 periment demonstrates that IVQ-CBM provides a mechanism not only for learning concepts but for
 1804 validating and refining the human knowledge base itself.

1806 Table 9: Performance comparison on the ISIC dataset before and after concept refinement. Guided by the
 1807 low assignment frequency in the IVQ codebook, replacing the dormant concept *Rough Texture* with *Irregular*
 1808 *Streaks* leads to consistent gains.

Model Setting	Concept Configuration	ACC (%)	BMAC (%)
Initial	Includes <i>Rough Texture</i>	90.11	86.22
Refined	Includes <i>Irregular Streaks</i>	90.75	87.12
<i>Performance Gain</i>		+0.64	+0.90

1818 L SENSITIVITY ANALYSIS OF COMMITMENT COST PARAMETER

1820 The commitment cost hyperparameter β in the IVQ loss (Eq. 4) serves a critical role in balancing
 1821 the strength of the regularization, specifically controlling how tightly the visual encoder’s output
 1822 is constrained to the learnable codebook prototypes. To empirically validate the model’s sensi-
 1823 tivity to this design choice, we conducted ablation experiments on three diverse datasets: ISIC
 1824 (Dermoscopy), SHIM (Chest X-ray), and BUSI (Ultrasound), evaluating a standard range of values
 1825 $\beta \in \{0.1, 0.25, 0.5, 1.0\}$.

1826 As summarized in Table 10, the model demonstrates remarkable robustness to variations in β . The
 1827 performance fluctuations in both Accuracy and BMAC are negligible (typically < 0.5%) across
 1828 all tested values. This stability suggests that the primary function of the IVQ loss is to provide a
 1829 structural constraint that prevents feature collapse. Our empirical results indicate that within the
 1830 examined range, the model is not sensitive to the precise magnitude of β , suggesting that the regu-
 1831 larization remains effective as long as the commitment cost is set to a reasonable non-trivial value.

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1859 Table 10: Sensitivity analysis of the commitment cost β on ISIC, SIIM, and BUSI datasets. The model shows
 1860 robust performance across a range of standard values, with the default setting ($\beta = 0.25$) highlighted in **bold**.

Commitment Cost (β)	ISIC (ACC / BMAC)	SIIM (ACC / BMAC)	BUSI (ACC / BMAC)
0.10	89.94 / 86.05	81.85 / 81.90	93.25 / 95.15
0.25 (Default)	90.11 / 86.22	82.01 / 82.01	93.59 / 95.38
0.50	90.02 / 86.14	81.92 / 81.95	93.41 / 95.22
1.00	89.85 / 85.92	81.70 / 81.65	93.10 / 94.95

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