Comparing Clinical and General LLMs on Knowledge Boundaries and Robustness

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Abstract

Large language models (LLMs) often know the correct answer internally even when their expressed output is wrong, which raises questions about how this knowledge is represented and whether domain adaptation changes it. We study how continued pretraining on domain corpora affects what a model knows and how reliably it can use this knowledge, with a focus on biomedical data. Comparing a general-purpose LLM with a clinical LLM obtained through continued pretraining on clinical text, we find that both retain similar levels of probe-accessible factual knowledge, yet the stability of self-monitoring signals is substantially reduced after domain pretraining. For example, the variance of error-detection performance nearly doubles in the biomedical model. An analysis of embedding geometry suggests that this reduced stability is associated with representations becoming more isotropic, with anisotropy decreasing from about 0.47 to 0.37. These results indicate that continued domain pretraining tends to reorganize rather than expand what the model knows, and can unintentionally weaken the consistency of error-detection signals, with implications for building reliable domain-adapted LLMs[1].

1 Introduction

Large language models (LLMs) have rapidly advanced the state of the art across a wide range of tasks. However, their tendency to produce hallucinations, meaning plausible yet factually incorrect statements, raises serious concerns about reliability, particularly in high-stakes domains such as medicine. Recent evidence indicates that exposing an LLM to new factual information during supervised fine-tuning can increase hallucination rates and slow learning: examples containing new knowledge are learned more slowly than those aligned with existing knowledge, and once acquired, hallucination rates grow roughly linearly with the proportion of novel facts in the fine-tuning data [1]. In addition, head-to-head evaluations on medical question answering show that domain-adapted LLMs rarely outperform general-purpose models; medical models win only about 12% of comparisons and are significantly worse in more than one third [2]. Taken together, these findings suggest that most factual knowledge is acquired during pre-training and that naive fine-tuning on biomedical corpora may, in fact, degrade factuality [1].

To mitigate hallucinations, a complementary line of work examines a model's hidden activations to understand what it knows [3, 4]. Early results show that a simple classifier trained on hidden states can distinguish true from false statements with 71–83% accuracy, outperforming probability-based heuristics [5]. More recent work on three-digit addition finds that lightweight probes can decode both

[1]Code will be released at https://github.com/Zephyr1022/knowledge-boundaries

the model's predicted answer and the correct answer from hidden states, even when the output is wrong; these probes can also predict whether the output will be correct with over 90% accuracy and can guide selective re-prompting [6]. Visualizations of hidden representations on true/false datasets reveal clear linear structure, and simple difference-in-means probes generalize across datasets while causally influencing the model's answer [7]. However, prior work mainly studies general-domain models on arithmetic or binary truth settings, and it remains unclear whether similar internal signals exist in clinical LLMs or for long-tail biomedical knowledge.

Two factors make the biomedical setting particularly challenging. First, biomedical knowledge is long-tailed: many facts appear in only a handful of documents. A model's ability to answer fact-based biomedical questions correlates strongly with how many pre-training documents mention the subject and object [8]. Even after applying knowledge-editing methods, performance on long-tail biomedical facts remains substantially lower than on high-frequency ones, partly because biomedical triples often follow one-to-many relations [9]. Second, hallucination detection is under-explored in medicine. The MedHallu benchmark shows that state-of-the-art models struggle to identify hallucinated answers in PubMedQA; even GPT-4o reaches only 0.625 F1 on the hardest category [10]. Moreover, hallucinations that are semantically close to the ground truth are the most difficult to detect [10], and general-purpose models outperform fine-tuned medical models on this task. These observations suggest that domain-specific fine-tuning may reorganize internal representations in ways that reduce the robustness of self-monitoring.

We present a lightweight and unified framework for biomedical knowledge probing and error detection. Given a factual triple template $T(s, r)$ with subject s and relation r, we first perform *external probing* by prompting the LLM to generate the corresponding object o and recording its top-k predictions. We then perform *internal probing* on residual-stream hidden states at the final subject token to decode (a) the object the model *believes* is correct and (b) a proxy for the ground-truth object. Building on prior work showing that simple probes can decode answers and detect errors from hidden states [5, 6, 11], we train logistic and MLP probes to determine whether the model's answer is correct. We evaluate this framework on both base and clinical LLMs (Mistral-7B, Llama-3, BioMistral) [12, 13, 14, 15], with a focus on long-tail biomedical triples where subject–object co-occurrences are infrequent [8, 9]. Finally, our probing approach contributes to mechanistic interpretability: analyzing linear directions in hidden states provides insight into how LLMs represent biomedical relations [7, 5, 16].

Motivated by these gaps, we ask: *Do clinical (domain-adapted) LLMs differ from general LLMs in how they internally represent and monitor factual knowledge?* We adapt the probing framework for arithmetic reasoning [6] to biomedical knowledge triples $\langle s, r, o \rangle$ and make three contributions:

1. **Cross-domain probing.** We develop simple circular, logistic, and MLP probes that decode both the model's predicted object and a proxy for the ground-truth object from hidden states at each layer. We find that, while both general and clinical models *know* latent biomedical facts internally, clinical models show much higher variance in error-detection signals across layers. This matters because a model cannot reliably detect or correct its own mistakes if the self-monitoring signal shifts from one layer to the next.
2. **Error detection and geometry.** We train lightweight classifiers to detect mismatches between the model's predicted and ground-truth objects, and analyze the geometry of hidden activations. General models exhibit more anisotropic and structured representations that support stable error-detection signals, whereas clinical models are more isotropic, making self-monitoring noisier and less reliable.
3. **Implications for safety.** We show that continued domain pretraining can reorganize internal representations in ways that weaken a model's ability to self-monitor. Lightweight probes provide a low-overhead tool for real-time error detection and highlight potential risks when deploying domain-adapted LLMs in clinical settings.

2 Related Work

Long-Tail Biomedical Knowledge. Biomedical knowledge follows a long-tailed distribution: many subject–object pairs occur in only a handful of training documents. An LLM's ability to answer fact-based questions depends strongly on how often the subject and object appeared during pre-training [8]. Kandpal et al. [8] show that even very large models struggle with rare biomedical

facts, requiring orders of magnitude more parameters to match performance on well-supported facts. While knowledge editing can inject missing facts, Yi et al. [9] find that edited models still perform substantially worse on long-tail biomedical triples than on high-frequency ones, in part because biomedical relations are often one-to-many, which limits edit generalization. These challenges motivate us to stratify our probing results by fact popularity to examine whether internal knowledge signals and error-detection cues differ between common and rare biomedical facts.

Mechanistic Interpretability. Mechanistic interpretability (MI) seeks to uncover the circuits, features, and directions inside neural networks that implement high-level behaviors. Recent work shows that truth-related signals are encoded in hidden activations and can be isolated with simple linear probes [7]; linear classifiers trained on hidden states can detect when a model is lying [5], and relational concept directions can be identified and used to causally steer model outputs [17]. We build on these insights by applying MI-inspired probing to domain-adapted biomedical models and analyzing how continued pretraining reshapes the geometry of internal representations.

Error Detection in LLMs. Reliable hallucination detection is critical for trustworthy LLM deployment. Azaria & Mitchell [5] showed that classifiers trained on hidden activations can distinguish true from false statements and provide more reliable confidence estimates than softmax probabilities. While many subsequent works explore probability- or consistency-based hallucination detectors, performance remains limited in the medical domain: on MedHallu, even GPT-4o achieves only moderate F1 scores, and hallucinations that are semantically close to the truth are the most difficult to detect [10]. We build on this line of work by comparing logistic, circular, and MLP probes for binary error detection and analyzing how their performance varies across layers and between general-purpose and clinical LLMs.

3 Method

We study biomedical triples $\langle s, r, o \rangle$ by prompting the model with a simple template $T(s, r)$ and extracting the residual–stream vector at layer l for the final subject token, $\mathbf{x}_l \in \mathbb{R}^d$. On this same representation $\mathbf{x}_l$, we train two decoders: an *internal* decoder that predicts the ground-truth object o (what the model "knows"), and an *external* decoder that predicts the model's own output $f_\theta(s, r)$ (what the model will "say"), following the probing framework for arithmetic reasoning of Sun, Stolfo & Sachan [6]. Because prior work shows that probe expressiveness influences what aspects of knowledge can be recovered [6], we use three complementary probe types: circular (captures low-dimensional geometric structure), logistic (linear and interpretable), and MLP (non-linear) to test whether our findings hold across probe capacities. We then convert the outputs of these decoders into a lightweight correctness score.

Probing Internal and External Knowledge. Both decoders share the same architecture and differ only in their training targets. We consider K candidate objects and use three lightweight probes applied to $\mathbf{x}_l$: (i) *circular*, which projects onto $(\mathbf{w}_1, \mathbf{w}_2)$, computes an angle $\theta = atan2(\mathbf{w}_2^\top \mathbf{x}_l,\ \mathbf{w}_1^\top \mathbf{x}_l)$, and predicts $\hat{k} = \lfloor (\theta/2\pi)\, K \rfloor$; (ii) *logistic*, which computes logits $\mathbf{z} = \mathbf{W}\mathbf{x}_l + \mathbf{b}$ and predicts $\hat{k} = \arg\max_i z_i$; and (iii) *MLP*, which computes $\mathbf{h} = \mathrm{ReLU}(\mathbf{W}_1\mathbf{x}_l + \mathbf{b}_1)$, then $\mathbf{z} = \mathbf{W}_2\mathbf{h} + \mathbf{b}_2$, and predicts $\hat{k} = \arg\max_i z_i$. We report *internal accuracy* for decoders trained to recover o and *external accuracy* for decoders trained to recover $f_\theta(s, r)$.

Probing for Error Detection. To detect when a model produces an incorrect biomedical fact, we apply three lightweight probes to the hidden activations: (i) a *Logistic* probe that provides a simple and interpretable linear classifier for detecting errors, (ii) an *MLP* probe that captures non-linear patterns in how correct and incorrect answers are represented, and (iii) a *Joint Circular Error Detector* that compares the model's internal belief and expressed answer using angular representations. The circular detector maps hidden activations to an angle $\theta = \mathrm{atan2}(w_1^\top x,\ w_2^\top x)$ and flags a triple as incorrect when the angular distance between the internal and external predictions exceeds a learned threshold. This yields an intuitive geometric signal for identifying errors, while keeping the probes lightweight and easy to interpret.

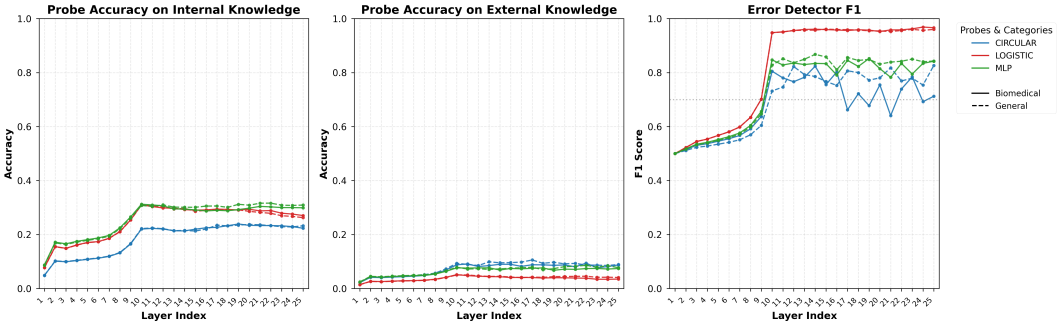

Figure 1: Layer-wise probe performance on general models (solid) and biomedical models (dashed). Left, internal Acc@10. Center, external Acc@10. Right, error-detector F1. Biomedical models exhibit notably higher variability in error detection at later layers despite similar average recall.

4 Experiment

We evaluate knowledge and error-detection signals in six large language models, consisting of three general-purpose models and their corresponding biomedical adaptations, across three datasets.

Language Models. We compare three open-source base models, Gemma-2-9B [18], Llama-3-8B [13], and Mistral-7B-Instruct-v0.1 [12], with their biomedical counterparts: Meditron3-Gemma2-9B [19], MMed-Llama-3-8B [20], and BioMistral-7B [14]. This pairing isolates the effect of domain-specific medical adaptation, which has been reported to not reliably improve factual recall or reduce hallucinations [2, 1].

Datasets and Prompts. We use three relation-based biomedical datasets. The first is MedLAMA, which contains UMLS triples from Meng et al. [21] for probing factual knowledge; we mark triples with fewer than ten PubMed co-occurrences as long-tail, following Kandpal et al. [8] and Yi et al. [9]. The second is a drug–symptom dataset from Berkowitz et al. [22] with 165 positive controls and 234 negative controls for assessing pharmacovigilance. The third consists of drug–drug interaction triples extracted from SemMedDB [23]. For each relation (e.g., "may treat"), we design a simple natural-language template such as "`[X] might treat [Y]`" to prompt the models; the full set of templates is provided in Appendix 1.

Evaluation Metrics. We assess how well a model can recall the correct object using Accuracy@K (Acc@1, Acc@5, Acc@10), which measures whether the correct answer appears within the model's top-K predictions. For example, Acc@10 counts a prediction as correct if the gold object o is included anywhere among the top-10 generated candidates for a triple $\langle s, r, o \rangle$. For error detection, we label a case as *correct* if the model's top-1 prediction matches o and *incorrect* otherwise, train lightweight probes on hidden states to predict this label, and report F1 scores. Following Meng et al. [21], we use "not appearing in the top-10" as the operational definition of an incorrect output.

To understand *where* knowledge becomes accessible inside the model, we apply probes across model layers: for layers $L \in \{1, \ldots, 25\}$, we extract residual-stream activations at the final subject token, train probes independently at each layer, and identify the depth with the best validation performance. Finally, we measure *retrieval failures*, cases where the model internally encodes the correct object but does not express it in the top-10 outputs, by training a probe to detect such failures and reporting F1 scores.

Experiment Results. Figure 1 presents layer-wise probe performance for general and biomedical models. Internal and external Acc@10 remain similarly low across both model types, indicating that continued domain pretraining does not add or remove probe-accessible knowledge. The key difference is *stability*: biomedical models show markedly higher layer-to-layer fluctuation in error-detection F1, especially in later layers (Table 2; e.g., circular probes SD $= 0.053$ vs. 0.027 for the corresponding general model). This matters because reliable self-monitoring requires a consistent signal over the forward pass; if the signal fluctuates with depth, downstream confidence-estimation or correction modules cannot rely on it.

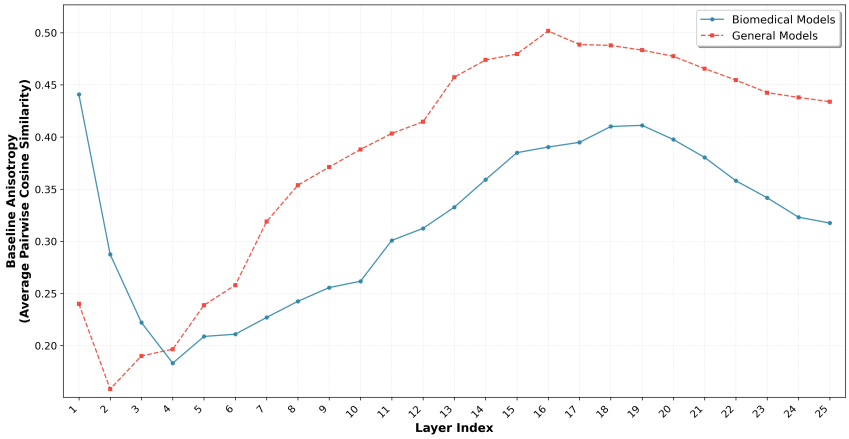

Figure 2: Baseline anisotropy across layers. General LLMs (red) show higher anisotropy. Clinical LLMs (blue) are more isotropic. Lower anisotropy coincides with more volatile error-detection.

To examine what may underlie this instability, we analyze representation geometry. Following Ethayarajh [24], we estimate *anisotropy* by measuring the average cosine similarity between random directions and layer-wise representations. As shown in Figure 2, general models are more anisotropic (peak ≈ 0.61) than their biomedical counterparts (peak ≈ 0.35). Prior work has argued that greater anisotropy reflects representations that are concentrated along a small number of dominant directions, which can make certain features easier to separate with simple linear readouts. In contrast, more isotropic representations are more uniformly spread, which can dilute these directions and make small differences harder to linearly decode.

Here, we observe that layers with lower anisotropy coincide with higher variability in probe performance (Figure 1, right). While this does not, by itself, establish causation, it suggests a plausible link: more isotropic representations may provide weaker or less stable linear signals for error detection, contributing to the observed volatility across layers. Taken together, these results support the view that continued domain pretraining tends to *reorganize*, rather than expand, probe-accessible knowledge, and that this reorganization can make internal error-detection signals less consistent. This aligns with recent findings that some domain-adaptation regimes can inadvertently increase hallucination rates.

5 Limitations and Conclusion

Our results show that general-purpose and biomedical LLMs contain similar amounts of probe-accessible knowledge, but their internal error-detection signals differ sharply in stability: across circular, logistic, and MLP probes, the biomedical model has nearly twice the across-layer standard deviation in error-detector F1 compared to the general model (Table 2). An isotropy analysis indicates a plausible mechanism: domain-specific fine-tuning reduces anisotropy, yielding more isotropic representations that are less amenable to simple linear separation of correct vs. incorrect states. Practically, this implies that fine-tuning reorganizes internal geometry without adding new knowledge and can make self-monitoring less reliable, consistent with reports that instruction tuning increases hallucination rates [1, 2]. As a simple diagnostic, we propose measuring the variability of internal error-detection signals to assess robustness. More broadly, our unified probing and error-detection framework links mechanistic interpretability to safety: by extracting both predicted and ground-truth objects from hidden states, lightweight probes act as oracles that anticipate hallucinations and, when plugged into re-prompting or abstention pipelines, improve reliability with minimal overhead. Although we focus on biomedical facts, the approach generalizes to other domains with long-tail knowledge and high-stakes decisions. Future work should study cross-model prediction [25], explore unsupervised clustering for richer error signals, and test whether stronger probes or representation editing can mitigate the variability introduced by domain-specific fine-tuning.

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Relation	Manual Prompt
may treat	[X] might treat [Y].
may prevent	[X] might prevent [Y].
adverse drug effect	The adverse effect of [X] is [Y].
interacts with	The [X] interacts with [Y].

Table 1: Templates $T(s, r)$ used to elicit $\mathbf{x}_l$. Here [X] is the subject s and [Y] is the object o.

Probe	Metric	Bio s.d.	Gen s.d.	Ratio
Circular	Acc@10	0.00730	0.00796	0.917
Circular	External_Acc@10	0.00441	0.00553	0.797
Circular	F1 (err. det.)	0.05287	0.02725	**1.940**
Logistic	Acc@10	0.00959	0.01311	0.732
Logistic	External_Acc@10	0.00460	0.00295	1.561
Logistic	F1 (err. det.)	0.00504	0.00353	**1.427**
MLP	Acc@10	0.00727	0.00477	1.526
MLP	External_Acc@10	0.00268	0.00473	0.567
MLP	F1 (err. det.)	0.01994	0.01292	**1.543**

Table 2: Across-layer standard deviations (s.d.) of probe metrics. Bio = biomedical model; Gen = general model. Larger s.d. indicates less stability across layers.

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A Experiments Compute Resources

All experiments were conducted on 4 NVIDIA H100 GPUs. Probe training and evaluation completed within approximately one day of wall-clock time.

B Prompt Templates and Layerwise Stability

This appendix documents (i) the minimal natural-language templates we use to render (s, r, o) tuples into prompts for extracting layer representations $\mathbf{x}\ell$, and (ii) the layerwise stability of three probe families. In Table 1, `[X]` is the subject s and `[Y]` is the object o; instantiating $T(s, r)$ yields the input from which we read $\mathbf{x}\ell$. Table 2 reports the standard deviation across layers for each metric; larger values indicate less stable signals over depth. Notably, error-detection F1 varies substantially more in the biomedical model.

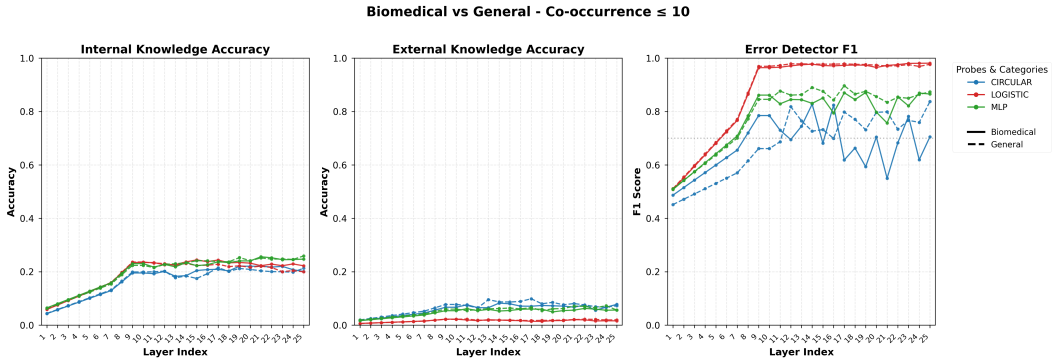

Figure 3: Layer-wise probe performance for low-frequency pairs (**co-occurrence** ≤ 10). Error detection is strong in deeper layers, with notably higher variability for the biomedical model (solid) relative to the general model (dashed).

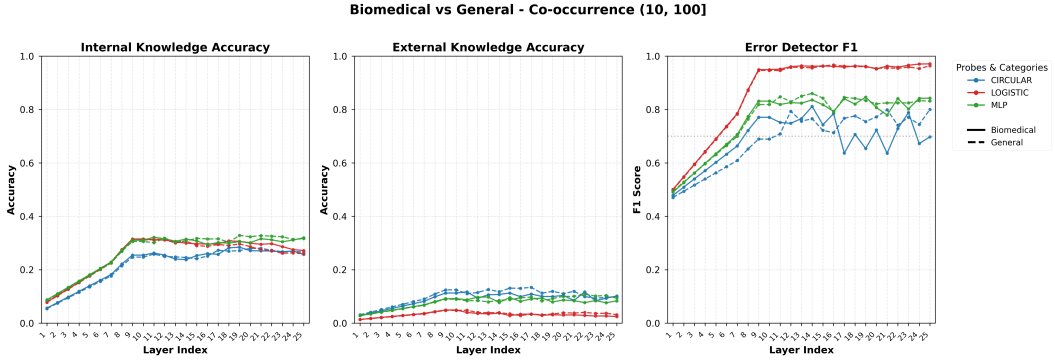

Figure 4: Layer-wise probe performance for **(10, 100]** co-occurrence. The stability gap persists: biomedical error-detection signals vary more across layers despite similar average recall.

C Additional Layer-wise Results by Co-occurrence

We stratify (s, o) pairs by corpus co-occurrence into four buckets (low to high frequency): ≤ 10, $(10, 100]$, $(100, 1000]$, and > 1000. For each bucket we plot layer-wise probe accuracy on internal and external knowledge (left/center) and error-detector F1 (right) for circular, logistic, and MLP probes. Across buckets, knowledge readout remains low while error detection strengthens with depth; the biomedical model shows consistently higher across-layer variability, especially in later layers.

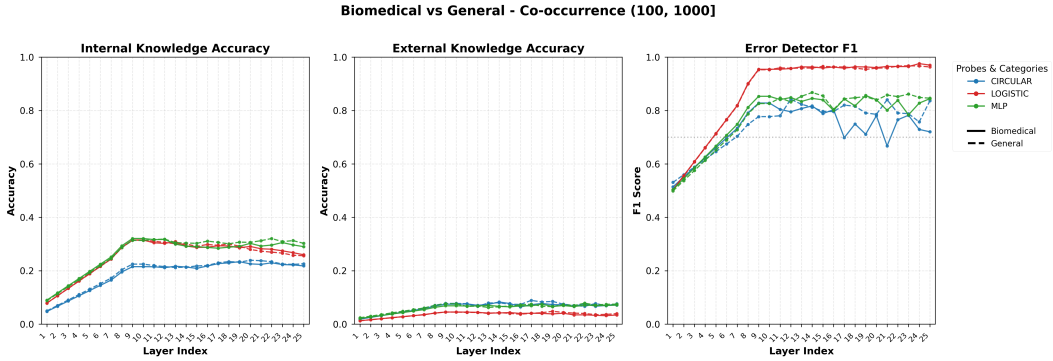

Figure 5: Layer-wise probe performance for **(100, 1000]** co-occurrence. General model (dashed) remains more stable across depth; biomedical model (solid) shows noisier F1 trajectories.

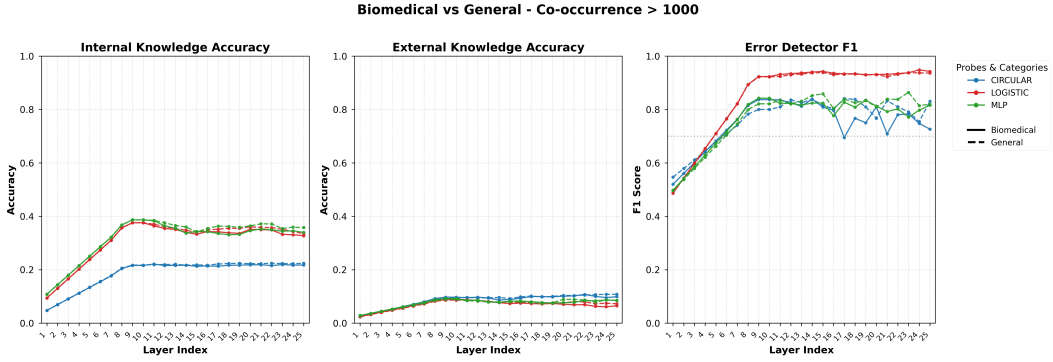

Figure 6: Layer-wise probe performance for high-frequency pairs (**co-occurrence** >1000). Trends hold with slightly smoother curves; biomedical error-detection variability remains elevated at later layers.

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   Question: Do the main claims made in the abstract and introduction accurately reflect the paper's contributions and scope?

   Answer: [Yes]

   Justification: The abstract and introduction state that domain-specific finetuning reorganizes internal representations without adding or removing probe-accessible knowledge, and that this reduces stability of error detection. These claims match the experiments and conclusions.

   Guidelines:

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   - The abstract and/or introduction should clearly state the claims made, including the contributions made in the paper and important assumptions and limitations. A No or NA answer to this question will not be perceived well by the reviewers.
   - The claims made should match theoretical and experimental results, and reflect how much the results can be expected to generalize to other settings.
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2. **Limitations**

   Question: Does the paper discuss the limitations of the work performed by the authors?

   Answer: [Yes]

   Justification: Section "Limitations and Conclusion" explicitly discusses that findings are limited to biomedical triples and that variability may arise from finetuning regimes. It also notes the scope (long-tail biomedical knowledge) and proposes future work.

   Guidelines:

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