Project 3b: Exploring Overtraining and Membership in ESM-2

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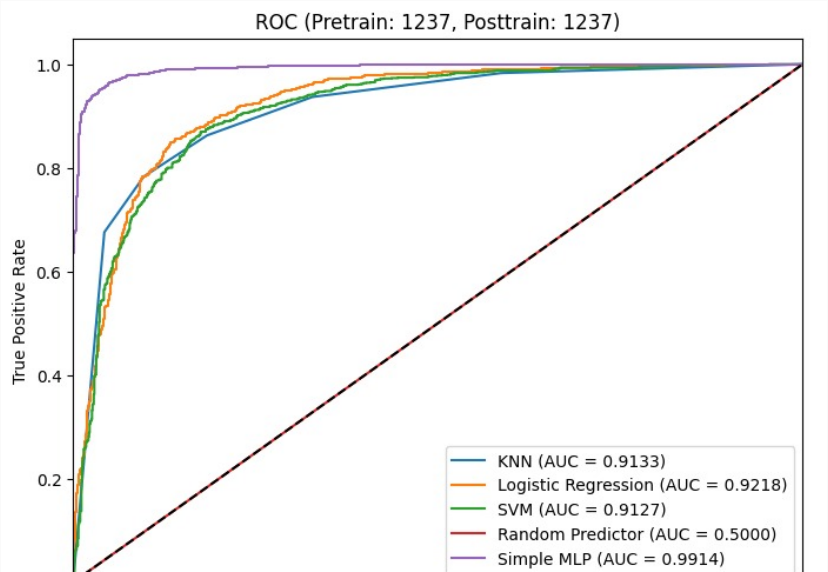
Membership attack recipe

- Training-time proxy: sequences sampled from $\sim$ UniRef50.
- Post-train proxy: newly discovered proteins (N)
- Goal: learn a detector that flags members vs. non-members

Results snapshot



Great job! 0.99 AUC!

Meta UR50D process (ESM-2 original)

- Meta samples 43M UniRef50 clusters, then pulls UniRef90 sequences within clusters; ∼65M unique sequences seen from 138M [1].
- The exact UR50D training file was never released; only the sampling recipe is public.

[1] Zeming Lin et al., *Evolutionary-scale prediction of atomic-level protein structure with a language model*. Science 379, 1123–1130 (2023). DOI:10.1126/science.ade2574.

What does that mean for MI?

- For any candidate protein, only $\approx 65/138$ chance it was actually in the ESM-2 train pool.
- Our MI probes risk targeting "maybe-seen" sequences $\Rightarrow$ unclear ground truth.
- What were we even measuring??

NVIDIA to the rescue

- Member proxy: NVIDIA UR50D train shards (T) — mirrors Meta recipe but reproducible/public.
- Non-member proxies:
  - New proteins (N) outside the train stream,
  - Validation shards (V) from NVIDIA split,
  - hard homologs from UniRef90 $\setminus$ T for .

Hardness ladder

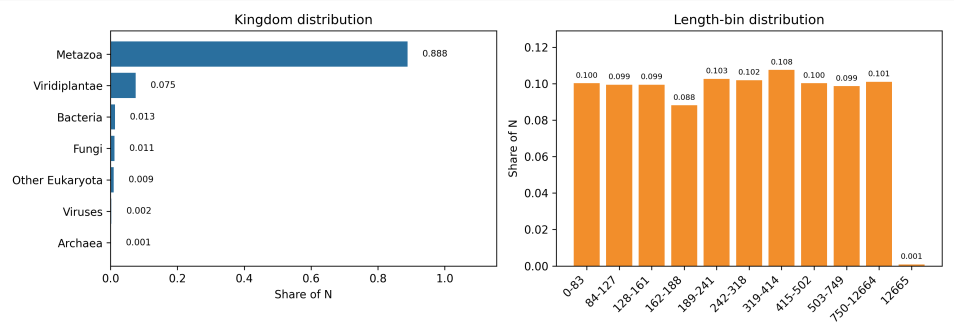
- Easy: $(S1, N)$ — $S1$ from T (train shards), N are new proteins; $|S1| = |N| = 1{,}237$.
- Medium: $(S2, S3)$ — $S2$ from T vs. $S3$ from V (val shards); equal size $K \approx 12\text{k}$.
- Hard: $(S4, U4)$ — $S4$ from T vs. $U4$ hard homologs from UniRef90 $\setminus$ T;

Each of the 3 pairs is then split 80/20 into train/test for the MI detector.

Sampling

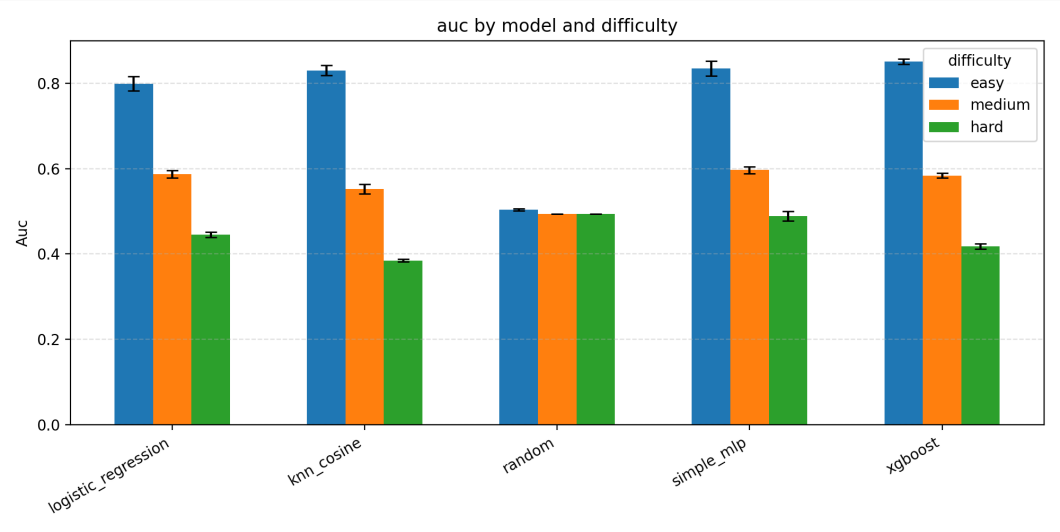
- Bin by (Kingdom, Length bin) on N.
- All sampled sets mirror the empirical N distribution to avoid easy shortcuts.
- Cluster-aware sampling (UR50) keeps representation balanced

N distribution (kingdom + length)

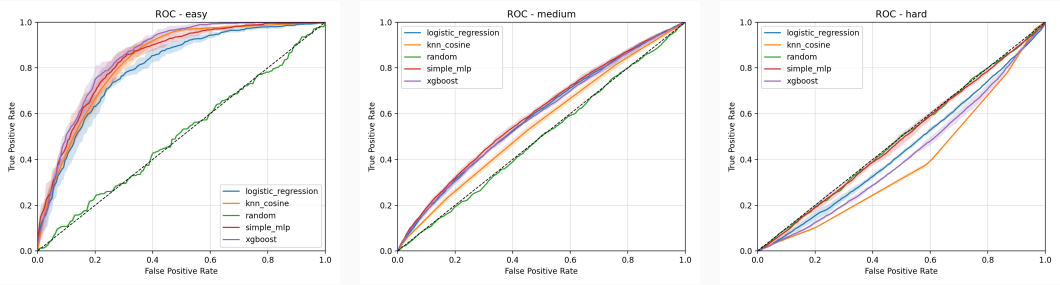


We use this empirical N distribution to set bin targets across T/V and UniRef90 sampling.

Accuracy (AUC)



ROC curves



Left: N vs S1 (easy). Middle: S2 vs S3 (medium). Right: S4 vs U4 (hard).

Idea from last week

- Results were not promising even on flawed data.
- 650M embeddings are not ready yet (NVIDIA released 8M, 650M, 3B) so we still didn't try them.
- Likely a waste of time.

sorry

Biggest success & next steps

Biggest success since last presentation

- Improved the data curation process.
- Identified the issue with using the Meta model.

Next steps (why/how they help)

- Finish the 650M embeddings to test larger capacity models.
- Try other MI methods and ideas from the first presentation.
- Improve the MLP model and explore additional approaches.