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# Inference-Time Alignment via Hypothesis Reweighting

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# Abstract

Chat assistants must handle diverse and often conflicting user preferences, requiring adapt-012 ability to various user needs. We propose a lightweight framework to address the general challenge of aligning models to user intent at 015 inference time. Our approach involves training an efficient ensemble, i.e., a single neural network with multiple prediction heads, each rep-018 resenting a different function consistent with the 019 training data. Our main contribution is HYRE, 020 a simple adaptation technique that dynamically reweights ensemble members at test time using a small set of labeled examples from the target distribution, which can be labeled in advance or actively queried from a larger unlabeled pool. The 025 computational cost of our training procedure is comparable to fine-tuning a single model, and thus scales to large pretrained backbones. We em-028 pirically validate HYRE in several target evalua-029 tion distributions. With as few as five preference 030 pairs from each target distribution, adaptation via HYRE surpasses state-of-the-art reward models on RewardBench at both the 2B and 8B parameter scales. 034

#### Introduction 1

Task specification-describing precisely what a machine learning model should do-is inherently iterative and fundamentally incomplete under any finite set of instructions or training examples. As models grow more powerful and are applied to increasingly complex and nuanced tasks, this problem arises in many forms, from spurious correlations in the data to conflicting user preferences. Consider a chatbot trained via Reinforcement Learning from Human Feedback (RLHF) (Siththaranjan et al., 2023) on a broad distribution of user preferences. Such models often perform adequately in aggregate but systemtically fail to address specific users' needs, since different individuals have distinct, sometimes contradictory, notions of desirable responses. Meeting these user-specific requirements necessitates rapid model adaptation with minimal supervision. However, existing adaptation strategies, such as prompt-based methods (Gao et al., 2020; Khattab et al., 2023; Yuksekgonul et al., 2024) and fine-tuning (Houlsby et al., 2019; Hu et al., 2021; Liu et al., 2024; Wu et al., 2024), can be computationally heavy, typically requiring multiple forward-backward passes or large-scale gradient updates. This renders them unsuitable for on-the-fly adaptation at test time.

To efficiently resolve ambiguity at test time, we draw on recent progress in efficient ensemble architectures (Osband et al., 2023). These methods let a single backbone network represent a broad range of plausible functions at a small overhead, capturing the different ways the model can interpret the training set. While prior work focuses largely on using ensembles for uncertainty estimation, we propose using them to disambiguate tasks in real time: by quickly assessing which members of the ensemble best match a new distribution, we can "pick the right interpretation" for that scenario.

We introduce Hypothesis Reweighting (HYRE), a two-step approach that scales to large models. First, we train an ensemble of function heads on top of a shared backbone, ensuring each head individually fits the training data. Next, at inference time, we gather a few labeled examples from the target distribution-either proactively queried or provided in advance-and measure each head's performance. We then reweight the ensemble using a generalized Bayesian update that favors the heads performing best on the adaptation set. Crucially, this update supports non-differentiable metrics like 0-1 error, and it requires only a single forward pass over the adaptation set, making it far more efficient than conventional fine-tuning.

We evaluate HYRE across over 20 target distributions including preference personalization tasks and benchmarks for response safety and usefulness. With just 1-5 adaptation examples, HYRE reweights a 100-head ensemble at negligible (< 1%) overhead, improving the state-of-the-art reward model by an average of 20% absolute accuracy across 32 tasks. Adaptation via HYRE also outperforms the state-

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Figure 1: Motivating observation: the ensemble average often performs worse than a single well-chosen member. This tendency is particularly pronounced further away from the training distribution. HYRE goes further than selecting the best head—it finds a continuous weighting of all heads.

Algorithm 1 HYRE (Inference Time)

- **Require:** Ensemble members  $f_{1..K}$ , unlabeled dataset  $x_{1..N}$ , query budget B
- 1: Initialize weights  $w \leftarrow [\frac{1}{K}, \dots, \frac{1}{K}]$ , query set  $Q \leftarrow \emptyset$ 2: for  $i \leftarrow 1$  to B do
- 3: (Optional) Query label  $y_n$  for  $\arg \max_n c(x_n)$  and add  $(x_n, y_n)$  to Q (Appendix F)
- 4: Compute accuracy  $\operatorname{acc}_k = \sum_{n \in Q} \operatorname{acc}(f_k, x_n, y_n)$ for each k
- 5: Update ensemble weight  $w_k \propto \exp(\operatorname{acc}_k + p)$  (Section 2)

### 6: end for

7: **Return** final weighted ensemble function  $f_w : x \mapsto \sum_{k=1}^{K} w_k f_k(x)$ 

of-the-art models on RewardBench (Lambert et al., 2024) at both the 2B and 8B parameter scales. These findings demonstrate that fast inference-time reweighting of a wellchosen ensemble can effectively adapt to new tasks with minimal supervision.

# 2 HYRE: Fast Inference-Time Ensemble Reweighting

In this section, we motivate and describe Hypothesis
Reweighting (HYRE), a simple and computationally efficient method for few-shot adaptation to new tasks. HYRE
dynamically adjusts the weights assigned to different ensemble members at test time based on a few labeled samples from the new task. HYRE leverages the ensemble's
diversity—each member representing a different function
that fits the training data—to efficiently adapt without retraining any model parameters.

Our method is motivated by Figure 1, which shows that the
ensemble average often performs substantially worse than
the best weighted ensemble. This tendency is particularly
pronounced further away from the training distribution.

Given an ensemble of K models  $f_1, \ldots, f_K$ , we aim to dynamically update their weights based on adaptation data. As a practical test-time assumption in settings where we cannot further train neural networks, we can think of the "best" model as being one of the K ensemble particles that performs best on the evaluation distribution. Starting with uniform weights  $w_k = \frac{1}{K}$ , we update them as new labeled data from  $P_{eval}$  becomes available.

The weighted ensemble prediction is  $f_w(x) = \sum_{i=1}^{K} w_i f_i(x)$ , where each  $w_i \ge 0$  and  $\sum_{i=1}^{K} w_i = 1$ . We measure each member's performance using a loss function  $l(f_k, x, y)$  and compute their cumulative loss on adaptation data  $\mathcal{L}(f_k, \mathcal{D}_{adapt}) = \sum_{(x,y) \in \mathcal{D}_{adapt}} l(f_k, x, y)$ . The weights are updated using a softmax on negative cumulative loss:

$$w_k = \frac{\exp(-\mathcal{L}(f_k, \mathcal{D}_{\text{adapt}}))}{\sum_{i=1}^{K} \exp(-\mathcal{L}(f_i, \mathcal{D}_{\text{adapt}}))}.$$
 (1)

As the loss  $l(f_k, x, y)$ , we use 0-1 error for classification and mean squared error for regression, though HYRE supports any performance metric since the weight update remains valid for non-differentiable functions. The complete adaptation procedure is summarized in Algorithm 1.

# **3** Experiments

We now empirically validate HYRE. We focus on three key questions: (1) Can HYRE effectively handle mild covariate shift? (2) Does HYRE scale to large models? (3) How robust and computationally efficient is HYRE? We describe the detailed setup for each experiment in the appendix.

### 3.1 Regression Data with Mild Covariate Shift

We evaluate HYRE on three UCI regression datasets (Kelly et al.)—Energy Efficiency, Kin8nm, and CCPP—using the protocol of Sharma et al. (2023): the top and bottom 5% of the data (sorted by mean input features) form an OOD target set, while the central 90% is split into train and validation sets. All methods employ 100 two-layer MLPs with

Model	Туре	Overall	Chat	Chat Hard	Safety	Reasoning
Tulu-2-DPO-70B	DPO	79.1	97.5	60.5	84.5	74.1
StableLM-2-12B-Chat	DPO	79.9	96.6	55.5	78.1	89.4
Claude-3 Sonnet (June 2024)	Gen	84.2	96.4	74.0	81.6	84.7
GPT-4 (May 2024)	Gen	84.6	96.6	70.4	86.5	84.9
GPT-4 (Aug 2024)	Gen	86.7	96.1	76.1	88.1	86.6
Gemini-1.5-Pro-0924	Gen	86.8	94.1	77.0	85.8	90.2
Skywork-Reward-Gemma-2-27B	Seq	94.3	96.1	89.9	93.0	98.1
INF-ORM-Llama3.1-70B	Seq	95.1	96.6	91.0	93.6	99.1
GRM-Gemma2-2B	Seq	88.4	93.0	77.2	92.2	91.2
+ Ours (uniform)	Seq	87.1	96.4	73.1	87.4	89.8
+ Ours (N=1)	Seq + HYRE	86.5	92.4	71.5	85.1	92.5
+ Ours (N=5)	Seq + HYRE	88.5	95.0	72.5	90.3	93.1
+ Ours (N=10)	Seq + HYRE	<b>89.7</b>	96.4	74.7	92.4	93.5
+ Ours (best head oracle) <sup>*</sup>	Seq + Oracle	91.8	97.2	80.0	96.2	94.2
+ Ours (best weight oracle) <sup>*</sup>	Seq + Oracle	93.1	98.3	83.4	96.7	94.9
Skywork–Llama-3.1-8B	Seq	94.0	94.7	88.6	92.7	96.7
+ Ours (uniform)	Seq	94.0	95.0	87.2	93.0	96.8
+ Ours (N=1)	Seq + HYRE	94.3	95.2	87.8	93.0	97.5
+ Ours (N=5)	Seq + HYRE	94.7	95.5	88.6	93.2	97.8
+ Ours (N=10)	Seq + HYRE	95.0	95.9	89.3	93.5	97.9
+ Ours (best head oracle) <sup>*</sup>	Seq + Oracle	96.4	98.3	91.2	95.7	98.4
+ Ours (best weight oracle)*	Seq + Oracle	97.2	99.2	93.0	96.5	98.8

\* Oracle methods show an upper bound on performance, using the test set.

Table 1: Accuracy across tasks in RewardBench. We report overall performance and breakdowns by task category for all models. HYRE
 improves upon the state-of-the-art models at the 2B and 8B parameter scales with as few as 1-5 labeled samples per distribution.

50 units each. As baselines, we consider a vanilla ensemble of independently trained models and MC Dropout (Gal & Ghahramani, 2016). We report the best-performing MC
Dropout results across all architectures. Results in Table 4
demonstrate that uniform ensembles perform strongly in
these OOD generalization settings and that HYRE consistently improves over the uniform ensemble.

# 147 **3.2** Scalable Personalization of Preference Models

148 **Experimental setup.** We evaluate personalization using 149 four sets of human preference benchmarks: Elix (Singh 150 et al., 2025), RewardBench (Lambert et al., 2024), PER-151 SONA (Castricato et al., 2024), and Anthropic HH (Bai 152 et al., 2022). Together, these benchmarks contain 32 153 datasets, each encoding a different aspect of human pref-154 erences. To train HYRE on preference data, we attach 155 Shared-Base ensemble heads to a pretrained 2B reward 156 model and fine-tune it on the UltraFeedback (Cui et al., 157 2023) dataset, a standard dataset for reward model training. We use two public finetune checkpoints of Gemma 2B 159 models, which achieve state-of-the-art performance on Re-160 wardBench at the 2B parameter scale, even outperforming 161 GPT-40 (Achiam et al., 2023). Refer to Appendix G for our 162 detailed setup. 163

We first evaluate the effectiveness of HYRE in adapting our reward model ensemble to new distributions at test time, comparing its performance to that of the original reward model. As shown in Figure 2, a simple uniform ensemble initially underperforms the original model, indicating that naive ensembling alone cannot ensure broad generalization. Nevertheless, HYRE quickly surpasses the baseline with just a few labeled examples per distribution. We show detailed dataset-level results in the appendix (Figure 9).

We compare HYRE against state-of-the-art reward models on the RewardBench leaderboard at both the 2B and 8B parameter scales. As shown in Table 8, HYRE—with only 1-5 labeled examples per distribution—exceeds the performance of many much larger reward models. We note that these reward models outperform strong generative reward models including Claude 3.5 Sonnet, GPT-4, and Gemini-1.5-Pro (Achiam et al., 2023; Anthropic, 2024; Team et al., 2024). This indicates that inference-time alignment can be a powerful alternative to naively scaling up reward models.

# 3.3 Comparison with Alternative Adaptation Methods

**Few-shot prompting.** We compare HYRE with few-shot prompting using GPT-40-mini on two datasets from Re-

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Figure 2: Average reward model accuracy as a function of adaptation set size. The dashed line shows the best available static 2B reward
 model for each dataset group. HYRE consistently outperforms the state-of-the-art reward model with as few as 1-5 examples per
 distribution.

Dataset	N=0	N=1	N=5	N=10	N=20	N=40	N=8
GPT-40-mini	N-Sho	t Prom	pting				
donotanswer	44.4	50.3	60.2	64.7	68.7	66.4	67.
refusals	79.4	<u>82.7</u>	80.5	82.2	82.1	78.0	82.
Llama-3.1-8B	8 N-Sho	t Prom	pting				
donotanswer	46.6	52.8	59.6	63.4	41.2	62.6	*
refusals	61.6	<u>82.4</u>	80.0	72.2	44.4	79.0	*
Llama-3.1-8B	B + HY	RE					
donotanswer	58.6	60.8	69.1	71.3			
refusals	88.9	90.0	94.0	95.2			

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Table 2: Comparison with few-shot prompting on two datasets from
RewardBench. (\*) exceeds Together AI API token limit. We see a
degradation in performance for both GPT-4o-mini and Llama-3.1-8B
as we increase the number of examples, whereas HYRE consistently
outperforms both across all sample sizes. HYRE provides reliable
test-time alignment, unlike few-shot prompting, which can degrade
with too much context.

195 wardBench. As shown in Table 2, HYRE consistently outperforms GPT-4o-mini across all sample sizes. Even 196 in the zero-shot setting, specialized reward models like 197 HYRE achieve higher performance than general-purpose language models like GPT-40-mini. Notably, we observe 199 that too many few-shot examples can actually harm perfor-200 mance, as seen with GPT-40-mini's performance drop after N=10 for donotanswer and N=20 for refusals. These results 202 203 demonstrate that specialized reward models with inferencetime adaptation can more efficiently leverage few-shot ex-204 amples than general-purpose language models. 205

206 Fine-tuning on target data. We compare HYRE against models fine-tuned on the helpful-base and harmless-base 208 training sets in the Anthropic-HH dataset. Results in Ta-209 ble 5 indicate that while targeted fine-tuning models 210 achieve higher performance in their respective target met-211 rics, they significantly reduce performance in the other. In 212 contrast, our HYRE-adapted ensemble not only increases 213 performance across each data distribution but also retains 214 or slightly improves performance in the other split. We 215 emphasize that we show fine-tuning performance only as 216 a point of comparison; fine-tuning a model for a target 217 distribution is usually too computationally expensive to 218 be done at inference time, and is thus not a practical 219

	donotanswer	xstest-sr	refusals
HYRE	w/ Cross-Entrop	y	
N=0	$58.60 \pm 4.93$	$82.80 \pm 2.43$	$88.90\pm3.25$
N=1	$62.53 \pm 4.00$	$85.78\pm3.06$	$92.49\pm3.28$
N=5	$62.57 \pm 1.88$	$87.38 \pm 1.26$	$93.17\pm2.19$
N=10	$62.25 \pm 1.71$	$87.51 \pm 1.19$	$93.21 \pm 1.77$
HYRE	w/ Accuracy		
N=0	$58.60 \pm 4.93$	$82.80\pm2.43$	$88.90\pm3.25$
N=1	$60.81 \pm 5.29$	$85.80\pm2.45$	$90.00\pm3.63$
N=5	$69.12\pm5.81$	$89.28 \pm 2.86$	$94.00\pm2.45$
N=10	$\textbf{71.32} \pm \textbf{6.33}$	$\textbf{90.32} \pm \textbf{3.20}$	$\textbf{95.20} \pm \textbf{2.32}$
Oracle	$76.54\pm2.35$	$90.32 \pm 1.91$	$99.50\pm0.87$

Table 3: Cross-entropy ablation experiment. We report average and std of accuracy (%) with varying numbers of adaptation examples (N) on three datasets. Using accuracy as the adaptation objective for HYRE significantly improves post-adaptation performance.

solution for inference-time alignment.

#### 3.4 Ablation Studies and Analysis

Ablation on reweighting criteria. We investigate the impact of using binary cross entropy instead of accuracy for reweighting. As shown in Table 3, using cross-entropy loss for reweighting significantly degrades performance across three representative RewardBench datasets. This is because cross-entropy loss is sensitive to outliers as it is unbounded from above, and thus can quickly overfit to a head.

**Computational overhead.** HYRE is designed to be efficient enough to be used at inference time. We use a single pre-trained backbone with K prediction heads, where each head is a very small MLP compared to the backbone. The parameter overhead is negligible: in our reward model experiments, 100 ensemble heads ( $5.5 \times 10^5$  parameters) add less than 0.03% to the parameter count of the Gemma-2B backbone ( $2.0 \times 10^9$  parameters). At inference time, reweighting requires only a single forward pass through the backbone and heads, with the subsequent weight calculation being minimal. The total cost increase in time and memory for using HYRE compared to the single base model is less than 1%.

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Inference-Time Alignment via Hypothesis Reweighting



Figure 3: **Overview of HyRE**. We train multiple prediction heads on a shared backbone. (Left) At inference time, we evaluate each head on a small labeled adaptation set drawn from the target distribution. (Right) We reweight the heads according to the sum of their accuracies on the adaptation set, and use the weighted ensemble to make predictions on new inputs.

# **A** Preliminaries

**Problem setup.** We consider a general supervised learning setting that includes classification, preference learning, and regression tasks. Let  $\mathcal{X}$  represent the input space and  $\mathcal{Y}$  the output space, with training distribution  $P_{\text{train}}$  and evaluation distribution  $P_{\text{eval}}$  defined over  $\mathcal{X} \times \mathcal{Y}$ . The training dataset  $\mathcal{D}_{\text{train}} = \{(x_i, y_i)\}_{i=1}^N$  consists of N examples drawn from  $P_{\text{train}}$ . We explore few-shot adaptation settings such as chatbot personalization, where a small adaptation set  $\mathcal{D}_{\text{adapt}} \sim P_{\text{eval}}$ only partially informs model performance under  $P_{\text{eval}}$ . The adaptation set  $\mathcal{D}_{\text{adapt}}$  can be labeled in advance or actively queried, and is much smaller than the training set  $(|\mathcal{D}_{\text{adapt}}| \ll |\mathcal{D}_{\text{train}}|)$ . For instance, in our main experiment,  $|\mathcal{D}_{\text{adapt}}| = 16$ compared to  $|\mathcal{D}_{\text{train}}| > 300,000$ , with adaptation occurring near-instantly after a single forward pass through the network.

- 469 1. Shared-Base Ensemble: A single neural network that parameterizes both the prior and ensemble components by sharing a common base.
  - 2. Epinet: A base network augmented by a small auxiliary network that introduces diversity via a learned index.

472 We train all ensemble members jointly by minimizing  $\sum_{k=1}^{K} \mathcal{L}(f_k, \mathcal{D}_{\text{train}})$  using SGD. These architectures have negligible 473 overhead—in our reward model experiments, 100 ensemble heads add only 550K parameters (0.03%) to the 2B-parameter 475 Gemma backbone. Please refer to Appendix H for architectural details.

# B When is Ensemble Reweighting Effective, and Why?

This section explores *the conditions under which ensemble reweighting is effective* through three illustrative examples: analyzing ensemble diversity through PCA, examining decision boundaries in classification, and comparing adaptation strategies.

Ensemble diversity reflects task ambiguity. We visualize how an ensemble's diversity reflects the axes of task ambiguity. We consider a synthetic regression task where the training data is sampled from a Gaussian Process (GP) prior. For target inputs  $x_1, \ldots, x_M$ , each ensemble member  $f_k$  produces predictions  $v_k \in \mathbb{R}^M$ . We perform Principal Component Analysis (PCA) on the prediction matrix  $V = (v_1, \ldots, v_K) \in \mathbb{R}^{M \times K}$  to yield components  $u_1, \ldots, u_m \in \mathbb{R}^M$  that capture the main variations between ensemble members.

488 Using an ensemble of 100 models trained on 7 inputs and evaluated on 1000 test inputs, we visualize the first three 489 principal components in Figure 4. Each component represents a distinct mode of variation while preserving smoothness 490 and fit to training data. Like wavelets, these components are localized in input space and form a basis for approximating 491 the ensemble. See Appendix J for further analysis of PCA applied to ensemble predictions.

Ensembles as diverse sharp decision boundaries. We build on an alternative interpretation of the Bradley-Terry model, where the model can be seen as representing a population of deterministic decision-makers. For items i and j with param-

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Inference-Time Alignment via Hypothesis Reweighting

Method	Energy	Kin8nm	ССРР	Model	Helpful	Harmless
MC Dropout	0.3033	0.6494	0.3761	Fine-Tune (Helpful)	73.03	32.59
Vanilla	0.1664	0.4514	0.2920	Fine-Tune (Harmless)	32.06	73.30
+ HYRE	0.1572 (-0.0092)	0.4498 (-0.0016)	0.2902 (-0.0018)	Pretrained RM	68.01	52.16
+ HyRF	0.1390 0.1345(-0.0051)	0.4823 0.4814 (-0.0009)	0.3000	Ensemble	66.34	50.90
Shared-Base	0.1508	0.5316	0.2976	+ HYRE (Helpful)	68.44	51.21
+ HYRE	0.1431 (-0.0077)	0.5314 (-0.0002)	0.2955 (-0.0021)	+ HYRE (Harmless)	64.24	57.66

Table 4: RMSE (lower is better) on test data with distribution shifts across three UCI datasets. We compare the performance of various ensemble architectures with test-time adaptation using HYRE. We find that for all three ensemble architectures, HYRE is consistently able to adapt to the distribution shift between training and test data.

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Table 5: Helpful vs harmless tradeoff. To establish an upper bound on performance, we fine-tune the reward model on the helpful and harmless datasets separately. **Reweighting an ensemble model with HYRE allows us to flexibly trade off between the two desiderata**.

eters  $\theta_i, \theta_j \in \mathbb{R}$ , the preference probability under the Bradley-Terry model is:

$$P(i \succ j) = \frac{e^{\theta_i}}{e^{\theta_i} + e^{\theta_j}} = P\left(\theta_i + \epsilon_i > \theta_j + \epsilon_j\right),\tag{2}$$

where  $\epsilon_i, \epsilon_j \sim \text{Gumbel}(0, 1)$ . Rather than a single stochastic decision-maker, the model can be seen as representing a population of deterministic decision-makers. Each decision-maker is characterized by a pair  $(\epsilon_i, \epsilon_j)$ , and makes sharp choices based on which among  $\theta_i + \epsilon_i$  and  $\theta_j + \epsilon_j$  is larger. The model's probabilistic behavior emerges from averaging across this population.

We hypothesize that diverse ensembles can learn such sharp decision boundaries from aggregate data across a population of annotators. To test this, we construct a synthetic preference learning task with conflicting labelers. We sample inputs  $(x_1, x_2)$  from  $[0, 1]^2$  and generate diverse linear decision boundaries  $w_1x_1 + w_2x_2 > 0$ , with  $w_1, w_2 \sim N(0, 1)$ . As shown in Figure 6, our ensemble quickly adapts to new decision boundaries, outperforming single models. The average ensemble prediction matches the "average" decision-maker, while individual members capture distinct boundaries. In particular, higher diversity coefficients for the prior network yields sharper boundaries per ensemble member. In Section 3, we show this enables rapid personalization in real-world preference tasks.

HYRE outperforms fine-tuning in low-data regimes. We compare HYRE to model fine-tuning on a synthetic binary 526 classification task. The training set contains inputs from  $[0,1]^5$  labeled as 1 and inputs from  $[-1,0]^5$  labeled as 0. The 527 target distribution is uniform over  $[-1,1]^5$  with a random linear decision boundary. Results in Figure 5 show that HYRE 528 outperforms fine-tuning in the low-data regime, achieving high accuracy with few queries. Fine-tuning eventually surpasses 529 reweighting with more data due to its higher capacity. This illustrates a bias-variance tradeoff: reweighting reduces variance 530 by restricting solutions to the ensemble's span, providing an advantage with limited data. Additionally, HYRE requires 531 only a single forward pass and negligible weight computation cost(1), making it especially suitable for large models and 532 533 resource-constrained settings.

Interpreting HYRE as generalized Bayesian inference. The weight update in (1) can be interpreted as a form of generalized Bayesian inference (Bissiri et al., 2016). Given an initial belief state  $\pi(w)$ , the updated belief after observing  $\mathcal{D}_{adapt}$ is:

$$\pi(w|\mathcal{D}_{\text{adapt}}) \propto \exp\left(-\mathcal{L}(w, \mathcal{D}_{\text{adapt}})\right) \pi(w),\tag{3}$$

which generalizes classical Bayesian inference by allowing arbitrary loss functions. Standard Bayes is recovered when l(w, x) is the negative log-likelihood. Under mild conditions like i.i.d. sampling, these updates are consistent and coherent: they converge to the optimal weighting and yield identical posteriors whether applied incrementally or in batches. For classification tasks, using 0-1 loss instead of log-likelihood provides more stable updates by avoiding outlier dominance (Izmailov et al., 2021). This makes HYRE particularly suitable for robust adaptation with non-differentiable metrics.

# C Related Work

**Ensembles and mixture-of-experts.** A long-standing theme in machine learning is using ensembles to improve predictive performance and uncertainty estimates when different members make independent mistakes (Krogh & Vedelsby, 1994;

Lakshminarayanan et al., 2017). This principle underlies Mixture-of-Experts (MoE) models, where a gating mechanism 550 551 dynamically selects experts (Jacobs et al., 1991; Jordan & Jacobs, 1994; Yuksel et al., 2012), recently scaled to large neural 552 networks via conditional activation (Fedus et al., 2022; Jiang et al., 2024; Lepikhin et al., 2020; Shazeer et al., 2017). 553 Our approach diverges from these methods in a fundamental way: rather than learning a routing function during training, 554 we perform adaptive reweighting of ensemble members at test time. Building on efficient ensemble methods with shared 555 backbones (Osband et al., 2023), we extend prior work on dynamic ensemble weighting (Jimenez, 1998; Shahhosseini et al., 556 2022), though these typically focus on differentiable loss-based objectives. In contrast, our method dynamically adjusts 557 ensemble weights based on non-differentiable evaluation metrics, allowing for more effective inference-time alignment.

558 Task underspecification and scalable alignment. In many machine learning tasks, the training data fails to fully define 559 desired model behavior (D'Amour et al., 2022; Geirhos et al., 2020). This challenge intensifies under limited data or 560 distribution shifts, where multiple hypotheses remain consistent with observations. Reinforcement learning faces similar 561 issues: reward specification is difficult in open-ended environments, and optimizing misspecified objectives can lead to 562 unintended behaviors (Gao et al., 2023; Pan et al., 2022; Skalse et al., 2022; Zhuang & Hadfield-Menell, 2020). Instead 563 of fully defining a task upfront, one can collect human demonstrations or pairwise preferences, framing task specification 564 as a cooperative game between agents and humans (Hadfield-Menell et al., 2016). Reinforcement Learning from Human 565 Feedback (RLHF) operationalizes this idea by using user preferences to guide post-training (Christiano et al., 2017; Ouyang 566 et al., 2022; Rafailov et al., 2024; Wirth et al., 2017), with some using ensembles (Ahmed et al., 2024; Coste et al., 2023; 567 Zhang et al., 2024). Recent work on pluralistic alignment (Sorensen et al., 2024) uses explicit domain labels or per-user 568 data to improve personalization (Barreto et al., 2025; Chen et al., 2024; Jang et al., 2023; Li et al., 2024; Poddar et al., 569 2024). However, these methods require explicit domain labels or per-user data. HYRE demonstrates that this additional 570 information is not necessary during training: a diverse ensemble trained on aggregate data can capture ambiguity, which 571 we can use to directly adapt to new users. Our experiments show this insight generalizes across several problem settings. 572

# **D** Discussion

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Our results demonstrate how efficient ensemble architectures can offer a practical path to inference-time alignment in large models. By attaching lightweight ensemble heads to a shared backbone, we can capture multiple plausible interpretations of the training distribution at negligible extra cost. Then, through a simple reweighting step that leverages just a handful of target-domain examples, the ensemble can effectively pick out the functions that align best with a new task. Our findings complement recent efforts that flexibly distribute compute at inference time (Brown et al., 2024; Snell et al., 2024). A natural next step is to close the loop by pairing our approach with a parameterization of the reward model that allows for direct behavior adjustments (Rafailov et al., 2024).

583 Our method currently relies on a small batch of labeled examples from the target distribution, and does not address single-584 sample or online streaming adaptation. Furthermore, while relying on minimal data, our reweighting still assumes that 585 the ensemble's functional diversity covers the new domain's core behaviors. Extending our framework to dynamically 586 expand or augment the ensemble as new tasks emerge is an exciting direction. Nevertheless, our results demonstrate that 587 lightweight ensembles with inference-time reweighting offer a promising and practical approach for aligning large models 588 at inference time.

Limitations. On the WILDS (Koh et al., 2021) benchmark, we observe limited gains over the uniform ensemble in four out of the five datasets we tested(see Table 9). We attribute this to insufficient functional diversity relevant to these specific natural distribution shifts. Thus, while HYRE significantly improves performance on personalization tasks, its effectiveness is limited on settings with more severe distribution shifts. We leave the exploration of how to best approach inference-time adaptation in such settings to future work.

# E Additional Experiments

**Effect of sampling strategy.** In Table 6, we compare the performance of different active learning criteria for selecting adaptation data points. We consider random sampling, BALD, and entropy, measuring their performance over 0 to 40 target examples. Across the acquisition of 40 examples, active learning methods (BALD and entropy) demonstrated slightly better performance compared to random sampling. Even random sampling consistently improves performance, indicating that HYRE can be used with data collected before inference without sacrificing performance.

603 WILDS experiments. We evaluate a trained Shared-Base ensemble, both with and without HYRE on the WILDS-





Figure 4: Principal component analysis of an ensemble of regression models. Left: Each gray line is the prediction of an ensemble member; the dashed line shows the ensemble mean. Right: The top three principal components of the ensemble's predictions reveal distinct axes of variation in predictive behavior. Searching among ensemble weights like HYRE acts as a strong inductive bias towards simple functions consistent with the training data.

Figure 5: HYRE vs. fine-tuning with different amounts of adaptation data. Despite using only a single forward pass, HYRE outperforms fine-tuning in low-data regimes.



Figure 6: Ensemble behavior under label ambiguity. (Left) We simulate conflicting preferences between labelers on a synthetic dataset. (Center) Ensemble-averaged predictions approximate the consensus, smoothing over disagreements. (Right) We measure the maximum agreement between an ensemble and a held-out labeler: increasing model diversity improves alignment with individual labelers.

Camelyon17 dataset (Koh et al., 2021), comparing against several representative methods for OOD generalization from the official WILDS benchmark. As shown in Table 7, test-time adaptation with HYRE consistently outperforms other methods that do not use domain labels and remains competitive with LISA (Yao et al., 2022), a strong method that leverages domain labels for targeted data augmentation. We also test Shared-Base ensembles on four additional WILDS datasets (CivilComments, Amazon, FMoW, iWildCam), but did not observe further improvements from ensemble reweighting via HYRE, as detailed in Table 9. Nonetheless, training a diverse ensemble consistently improved OOD generalization in these datasets. We attribute the limited benefit of ensemble reweighting in these cases to some natural distribution shifts behaving similarly to in-distribution data in terms of task underspecification. For further discussion on the conditions that can make a single model outperform the ensemble, see Appendix B.

We further compare the performance of HYRE with few-shot fine-tuning with the same amount of adaptation data. We evaluate both HYRE and fine-tuning with  $\{4, 8, 16, 32\}$  datapoints from the OOD test set. Our results in Figure 7 show that ensemble reweighting outperforms fine-tuning in the low-data regime (4 and 8) examples, and fine-tuning eventually surpasses the performance of ensemble reweighting.

# **F** Active Learning Details

We also consider an active learning setup in which the N datapoints to label for HYRE are chosen at test time from a larger unlabeled pool of data. Rather than choosing all datapoints at once, we choose one datapoint at the time based on one of the following three criteria:

Inference-Time Alignment via Hypothesis Reweighting

Method	N=0	N=1	N=5	N=10	N=20	N=40
HYRE + Random	84.40	85.33	86.97	87.34	88.01	88.83
HYRE + Entropy	84.40	84.25	86.73	87.54	88.60	89.76
HYRE + BALD	84.40	84.28	87.13	87.78	88.60	88.99

Table 6: Accuracies on RewardBench with different datapoint selection strategies. While active sampling methods perform slightly

667 better, even random sampling consistently improves performance with the HYRE reweighting process.

Algorithm	DL	Test Acc
IRM	0	64.2 (8.1)
CORAL	0	59.5 (7.7)
Group DRO	0	68.4 (7.3)
Fish	0	74.7 (7.1)
LISA	0	77.1 (6.9)
ERM	Х	70.3 (6.4)
Evading	Х	73.6 (3.7)
Ensemble	Х	71.5 (3.4)
Ensemble + HYRE	Х	<b>75.2</b> (5.3)

Table 7: Test set accuracy on Camelyon17. HYRE achieves competitive performance without using domain labels (DL).

- Entropy (classification):  $H\left(\sum_{h=1}^{H} w_h f_h(x)\right)$ . This criterion selects datapoints where the weighted ensemble is most uncertain, promoting the exploration of ambiguous regions.
- **BALD** (classification):  $H\left(\sum_{i=1}^{H} w_i f_i(x)\right) \sum_{i=1}^{H} w_i H(f_i(x))$ . BALD considers both ensemble uncertainty and disagreement among members, balancing exploration and exploitation (Gal et al., 2017; Houlsby et al., 2011).
- Variance (regression):  $\sum_{i=1}^{H} w_i (f_i(x) \bar{f}(x))^2$ , where  $\bar{f}(x) = \sum_{i=1}^{H} w_i f_i(x)$ . This criterion focuses on points where ensemble predictions have the highest variance, which is a good indicator of uncertainty in regression tasks.

Each of these criteria can be computed quickly. Because the belief states w has a closed-form update that can be computed very quickly, we can efficiently recompute the next best data point after each active label query.

We note that the first criterion (Entropy) does not distinguish between so-called aleatoric uncertainty and epistemic uncertainty. Therefore, this criterion is susceptible to the "noisy TV problem", where an agent fixates on a source of uncertainty that cannot be resolved (Burda et al., 2018; Laskin et al., 2021). In practice, we find that HYRE is robust to the choice of active learning criterion, and even random selection is effective at adapting to the target distribution.

# G Experimental Details

Unless specified otherwise, we use the following configuration for the ensemble networks. We use an ensemble of 100 models. The learnable and prior networks are each a one-hidden-layer MLP with 128 units. For the epinet, the epistemic index is 10-dimensional. For ensemble reweighting via HYRE, we use 32 examples from the target dataset, actively queried based on the BALD (classification) or Variance (regression) criterion. We found that final performance is not very sensitive to the choice of active learning criterion, and even random sampling resulted in consistent benefits.

**WILDS.** We closely follow the reference WILDS implementation for each dataset (Koh et al., 2021), including the choice of backbone, learning rate, and weight decay. We briefly describe the baseline methods used in our experiments:

CORrelation ALignment (Sun et al., 2017, CORAL): CORAL is an unsupervised domain adaptation method that aligns the second-order statistics (covariances) of source and target feature distributions.

Inference-Time Alignment via Hypothesis Reweighting



Figure 7: Comparison of HYRE and few-shot fine-tuning on the Camelyon17 OOD test set. HYRE outperforms fine-tuning in the low-data regime despite requiring significantly less computational cost.

- Invariant Risk Minimization (Arjovsky et al., 2019, IRM): IRM aims to learn data representations that capture invariant correlations across multiple training distributions.
- Group Distributionally Robust Optimization (Sagawa et al., 2019, Group DRO): Group DRO seeks to minimize the worst-case training loss over predefined groups within the data.
- Fish (Shi et al., 2021): Fish is a domain generalization technique that approximates inter-domain gradient matching by maximizing the inner product between gradients from different domains.
- LISA (Yao et al., 2022): LISA builds on MixUp and selectively interpolates data samples to achieve domain invariance.

LLM Preference Learning We finetune three reward model checkpoints (Yang et al., 2024):

- https://huggingface.co/Ray2333/GRM-Gemma-2B-rewardmodel-ft
- 746 https://huggingface.co/Ray2333/GRM-Gemma2-2B-rewardmodel-ft
  - https://huggingface.co/Skywork/Skywork-Reward-Llama-3.1-8B-v0.2

Our ensemble architecture uses these networks as the backbone, and small MLPs for the learnable and prior networks which take the backbone's final embedding as input. We use the TRL codebase for reward model training (von Werra et al., 2020). We train with bfloat16 mixed precision. We use a learning rate of 0.0001, no weight decay, a batch size of 16, and train for 5000 steps. We consider four collections of preference datasets:

- Elix (Singh et al., 2025) is inspired by the "Explain like I'm 5" subreddit. It consists of questions answered at five educational levels: elementary, middle, high, college, and expert. Preference pairs are created by scoring how different pairs of GPT-4 generated responses meet the expected comprehension at each level.
- RewardBench (Lambert et al., 2024) is a suite of 27 preference datasets designed to test reward models on a broad spectrum of tasks, including chat quality, safety, reasoning, coding, and refusal handling. In our aggregate results Figure 2, we drop datasets with less than 100 examples. In our RewardBench experiments Table 8, we use all datasets to ensure a fair comparison with existing methods.
- **PERSONA** (Castricato et al., 2024) contains preference data derived from a collection of synthetic personas with diverse demographic attributes and values. We sample 10 personas and treat each as a target distribution. Further details are in Appendix K.
- Anthropic HH (Bai et al., 2022) contains human-labeled preferences focused on helpfulness and harmlessness. We use the helpfulness-base and harmlessness-base splits as evaluation distributions to measure the tradeoff between the two objectives.

Inference-Time	Alignment	via Hypothesis	Reweighting
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Model	Туре	Overall	Chat	Chat Hard	Safety	Reasoning
Mixtral-8x7B-Instruct-v0.1	DPO	77.6	95.0	64.0	72.6	78.7
LLaMA-3-Tulu-2-DPO-70B	DPO	77.2	96.4	57.5	74.9	80.2
Tulu-2-DPO-13B	DPO	76.7	95.8	58.3	79.5	73.2
Tulu-2-DPO-70B	DPO	79.1	97.5	60.5	84.5	74.1
StableLM-2-12B-Chat	DPO	79.9	96.6	55.5	78.1	89.4
Claude-3 Sonnet (June 2024)	Gen	84.2	96.4	74.0	81.6	84.7
GPT-4 (May 2024)	Gen	84.6	96.6	70.4	86.5	84.9
GPT-4 (Aug 2024)	Gen	86.7	96.1	76.1	88.1	86.6
Gemini-1.5-Pro-0924	Gen	86.8	94.1	77.0	85.8	90.2
Skywork-Reward-Gemma-2-27B	Seq	94.3	96.1	89.9	93.0	98.1
INF-ORM-Llama3.1-70B	Seq	95.1	96.6	91.0	93.6	99.1
GRM-Gemma-2B	Seq	84.5	89.4	75.2	84.5	88.8
+ Ours (uniform)	Seq	84.5	88.6	72.9	83.7	89.8
+ Ours (N=1)	Seq + HYRE	85.3	88.5	72.7	85.5	91.4
+ Ours (N=5)	Seq + HYRE	86.4	90.3	72.6	89.1	91.4
+ Ours (N=10)	Seq + HYRE	87.2	90.4	72.5	90.0	92.3
+ Ours (best head oracle)*	Seq + Oracle	88.6	91.1	78.1	91.9	92.3
+ Ours (best weight oracle) <sup>*</sup>	Seq + Oracle	90.0	92.3	81.8	92.5	93.1
GRM-Gemma2-2B	Seq	88.4	93.0	77.2	92.2	91.2
+ Ours (uniform)	Seq	87.1	96.4	73.1	87.4	89.8
+ Ours (N=1)	Seq + HYRE	86.5	92.4	71.5	85.1	92.5
+ Ours (N=5)	Seq + HYRE	88.5	95.0	72.5	90.3	93.1
+ Ours (N=10)	Seq + HYRE	<b>89.7</b>	96.4	74.7	92.4	93.5
+ Ours (best head oracle) <sup>*</sup>	Seq + Oracle	91.8	97.2	80.0	96.2	94.2
+ Ours (best weight oracle) <sup>*</sup>	Seq + Oracle	93.1	98.3	83.4	96.7	94.9
Skywork–Llama-3.1-8B	Seq	94.0	94.7	88.6	92.7	96.7
+ Ours (uniform)	Seq	94.0	95.0	87.2	93.0	96.8
+ Ours (N=1)	Seq + HYRE	94.3	95.2	87.8	93.0	97.5
+ Ours $(N=5)$	Seq + HYRE	94.7	95.5	88.6	93.2	97.8
+ Ours (N=10)	Seq + HYRE	95.0	95.9	89.3	93.5	97.9
+ Ours (best head oracle)*	Seq + Oracle	96.4	98.3	91.2	95.7	98.4
+ Ours (best weight oracle)*	Seq + Oracle	97.2	99.2	93.0	96.5	98.8
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\* Oracle methods show an upper bound on performance, using the test set.

Table 8: Accuracy across tasks in RewardBench. We report overall performance and breakdowns by task category for all models. HYRE improves upon the state-of-the-art models at the 2B and 8B parameter scales with as few as 1-5 labeled samples per distribution.

For the few-shot prompting experiments, we use GPT-40-mini. For each number of "shots"  $N \in \{0, 1, 5, 10, 20, 40, 80\}$ , we sample 1000 examples from the target distribution and use them to prompt GPT-40-mini.

# H Diverse Ensemble Architectures

We describe the diverse ensemble architectures used in our experiments. Each architecture is designed to parameterize an ensemble of H models, whose outputs are later combined to form an ensemble prediction. The key goal of these architectures is to produce diverse predictions across the ensemble at a low computational cost.

All architectures are trained end-to-end by minimizing the sum of a standard loss function (cross-entropy for classification,

Inference-Time Alignment via Hypothesis Reweighting

		CivilComments	Amazon	FMoW	iWildCam
Algorithm	DL	Worst-Group Acc	10% Acc	Worst-Reg Acc	Macro F1
IRM	0	66.3 (2.1)	52.4 (0.8)	32.8 (2.09)	15.1 (4.9)
IRMX	0	73.4 (1.4)	-	33.7 (0.95)	26.7 (1.1)
IRMX (PAIR)	0	74.2 (1.4)	-	35.4 (1.3)	27.9 (0.9)
CORAL	0	65.6 (1.3)	52.9 (0.8)	32.8 (0.66)	32.7 (0.2)
Group DRO	0	70.0 (2.0)	53.3 (0.0)	31.1 (1.66)	23.8 (2.0)
DFR	0	72.5 (0.9)	-	42.8 (0.42)	-
Fish	0	75.3 (0.6)	53.3 (0.0)	34.6 (0.18)	22.0 (1.8)
LISA	0	72.9 (1.0)	54.7 (0.0)	35.5 (0.81)	-
ERM	Х	56.0 (3.6)	53.8 (0.8)	31.3 (0.17)	30.8 (1.3)
Shared-Base	Х	58.1 (2.2)	54.2 (0.6)	32.8 (0.4)	30.9 (0.8)
Shared-Base + HYRE	Х	58.1 (0.2)	54.2 (0.6)	32.8 (0.4)	31.0 (0.8)

Table 9: Performance on additional WILDS benchmark datasets. The DL column indicates whether the algorithm uses domain labels. Using a Shared-Base ensemble consistently results in gains in OOD generalization metrics over prior methods. However, we observe no further benefits from reweighting the ensemble via HYRE on these datasets.

MSE for regression) over all ensemble members:

$$\sum_{h=1}^{H} \mathcal{L}\left(f_h(x), y\right). \tag{4}$$

Here, x is an input example, y is the true label, and  $f^i$  is the *i*-th ensemble member. While each individual model minimizes the training loss, we want the ensemble members to extrapolate to unseen data in diverse ways. The specific ensemble parameterizations, which we describe below, are designed to achieve this goal.

#### H.1 Vanilla Ensemble

A vanilla ensemble consists of H independently initialized and trained neural networks with identical architectures. Each network  $f_h$  takes an input x and produces an output  $f_h(x)$ . No parameters are shared. While simple to implement, this approach scales poorly as H increases since both memory and computation scale linearly with H.

### H.2 Shared-Base Ensemble

We propose a scalable neural network architecture that can represent thousands of diverse ensemble members. The network outputs H real-valued predictions in parallel, with the output space being  $\mathbb{R}^H$ . The architecture comprises a frozen prior network  $f_p$  and a learnable network  $f_{\theta}$ , both of which produce outputs of shape  $\mathbb{R}^H$ . Although the architectures of  $f_p$  and  $f_{\theta}$  are identical in our experiments, this is not a requirement.

For a given input x, the network output is

$$f^{p}(z) + f^{\theta}(z) = \begin{bmatrix} f_{1}^{p}(z) + f_{1}^{\theta}(z) \\ f_{2}^{p}(z) + f_{2}^{\theta}(z) \\ \vdots \\ f_{H}^{p}(z) + f_{H}^{\theta}(z) \end{bmatrix} \in \mathbb{R}^{H}$$
(5)

where each prediction  $f_i^p(z) + f_i^\theta(z)$  is compared against the ground-truth label y. The parameters of  $f^p$  are fixed at initialization and do not change during training; the parameters of  $f^\theta$  are learnable.

Using the frozen prior network  $f^p$  is crucial to the diversity in this architecture. If we were to only train  $f^{\theta}$ , the ensemble of the *H* predictions would have low diversity due to co-adaptation. To understand why this architecture produces a diverse ensemble, note that each learnable head solves a shifted task determined by the corresponding prior network head. Since we undo this shifting when producing the final prediction, we can view the different learnable heads as solving a different yet equivalent task.

## 880 H.3 Epinet

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The epinet architecture combines a base model  $f^{\text{base}} : \mathcal{X} \to \mathbb{R}^K$  with an epistemic network  $f^{\text{epi}} : \mathcal{Z} \times \mathbb{R}^{d_{\text{ftrs}}} \times \mathcal{X} \to \mathbb{R}^K$ . The base model can be any regular neural network, including a large pretrained model, and is used to extract features through a feature extractor  $\phi : \mathcal{X} \to \mathbb{R}^{d_{\text{ftrs}}}$ . Here,  $d_{\text{ftrs}}$  is the dimension of the extracted intermediate representations.

The epistemic network (epinet) is composed of two parts:

- A frozen prior network f<sup>epi-frozen</sup> : X → ℝ<sup>1,...,d<sub>index</sub>×K. The parameters of this network are fixed at initialization and do not change during training.
  </sup>
- A trainable network  $f^{\text{epi-trainable}} : \mathcal{Z} \times \mathbb{R}^{d_{\text{ftrs}}} \times \mathcal{X} \to \mathbb{R}^{K}$ .

Given an epistemic index  $z \in \mathbb{R}^d$  and input  $x \in \mathcal{X}$ , we compute the model output as:

$$f(z,x) = f^{\text{base}}(x) + v f^{\text{epi-frozen}}(x) \cdot z + f^{\text{epi-trainable}}(z,\phi(x),x) \cdot z$$
(6)

where  $\cdot$  is the dot product and  $v \in (0, \infty)$  is the so-called prior scale. At each step, we sample multiple epistemic indices z to form an ensemble, i.e.,  $f_1(x), \ldots, f_H(x) = f(z_1, x), \ldots, f(z_H, x)$ . This architecture efficiently generates diverse predictions by sampling different epistemic indices z while leveraging a potentially large pretrained base model.

# 900 I Repulsion vs Random Priors for Diversity

A line of prior work use repulsion for enforcing diversity between ensemble members. The high-level idea is to add a regularization term to the loss function that is minimized when the ensemble members are sufficiently "different" according to some distance metric. For example, Teney et al. (2022) uses a repulsion term that maximizes the cosine distance between the gradient of each ensemble member, and Lee et al. (2023) maximizes the mutual information of ensemble predictions on OOD inputs. While these techniqueshave seen success in certain settings, our early experiments indicate that such explicit regularization often results in a suboptimal ensemble. The repulsion term can overpower the learning signal in the training data, leading to ensemble members that are diverse but inaccurate.

909 In contrast, diversification via random priors (Osband et al., 2023) provides a more balanced approach. The key idea is to 910 initialize each ensemble member with a different random prior function which is fixed throughout training. This introduces 911 diversity from the start without explicitly optimizing for it during training. This approach maintains diversity without 912 sacrificing accuracy on the training data, and the degree of diversification is easily controlled by scaling the prior functions.

# J Function-Space Dimensionality Reduction

Here, we expand on the idea of PCA on ensemble predictions. A central challenge with large model ensembles is understanding the commonalities and differences among the individual models. The high-level idea is that PCA applied to ensemble predictions reveals the major direction of variation within an ensemble of models. This dimensionality reduction allows us to clearly interpret model behaviors and identify groups of related datapoints Additionally, PCA enables the generation of new functions with similar statistical properties by parameterizing a low-rank Gaussian distribution in the joint prediction space, which we can sample from.

# J.1 Motivating Example

Consider three models  $f_1, \ldots, f_3$  and five inputs  $z_1, \ldots, z_5$ . Denoting each model's predicted probability for an input as  $p_{nh} = \sigma(f_h(z_n)) \in [0, 1]$ , assume that the matrix of predictions is

$$\begin{pmatrix} p_{11} & p_{12} & p_{13} & p_{14} & p_{15} \\ p_{21} & p_{22} & p_{23} & p_{24} & p_{25} \\ p_{31} & p_{32} & p_{33} & p_{34} & p_{35} \end{pmatrix} = \begin{pmatrix} 1 & 0 & 1 & 0 & \frac{1}{2} \\ 0 & 1 & \frac{1}{2} & \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} & 0 & 1 & \frac{1}{2} \end{pmatrix}.$$
(7)

Each row of this matrix shows one model's prediction on the entire pool of inputs, and each column shows every model's prediction on a single input. We can analyze such a matrix of predictions on three levels, each revealing increasing amounts of structure within the ensemble:

**Level 1: Per-sample ensemble uncertainty.** We can first compute the average prediction  $\bar{p}(x) = \frac{1}{H} \sum_{h} p_{nh}$  for each datapoint. For the predictions in (7), the average prediction is  $\bar{p}(x) = \frac{1}{2}$  for every input x, and thus the collection of models may be viewed as equally uncertain about each of the 5 inputs. This is the measure of ensemble uncertainty commonly used for ensembles (Lakshminarayanan et al., 2017).

**Level 2: Per-sample disagreement.** We can further account for the amount of disagreement among ensemble members for each datapoint. Note that for the four inputs  $z_1, z_2, z_3, z_4$ , there is strong disagreement between two functions where one predicts 0 and the other predicts 1. This is not true of  $z_5$ , where all functions predict  $\frac{1}{2}$ . Uncertainty metrics that take disagreement into account, such as the BALD criterion (Houlsby et al., 2011), will reveal that the ensemble is more uncertain about  $z_1, z_2, z_3, z_4$  than it is about  $z_5$ .

**Level 3: Joint predictions.** First, note that the two approaches above discard all information about which ensemble member made which individual prediction for a given input, by (1) averaging all predictions or (2) considering only the unordered set of predictions. There is additional structure to the differences among ensemble members that we can extract by considering the joint predictions, i.e., viewing each column of (7) as an object in itself. The pair of inputs  $(z_1, z_2)$ are closely related since they deviate from the ensemble prediction in the same "direction" in the joint prediction space ( $\mathbb{R}^H$ ). We can make the same observation about the pair  $(z_3, z_4)$ . To see this structure more clearly, consider the matrix of deviations from the ensemble prediction  $\delta_{nh} = p_{nh} - \frac{1}{H} \sum_h p_{nh}$ :

$$\begin{pmatrix} \delta_{11} & \delta_{12} & \delta_{13} & \delta_{14} & \delta_{15} \\ \delta_{21} & \delta_{22} & \delta_{23} & \delta_{24} & \delta_{25} \\ \delta_{31} & \delta_{32} & \delta_{33} & \delta_{34} & \delta_{35} \end{pmatrix} = \frac{1}{2} \begin{pmatrix} 1 & -1 & 1 & -1 & 0 \\ -1 & 1 & 0 & 0 & 0 \\ 0 & 0 & -1 & 1 & 0 \end{pmatrix}.$$
(8)

This clearly shows that the vector of joint deviations  $(\delta_{11}, \delta_{12}, \delta_{13})$  is the negative of that of  $(\delta_{21}, \delta_{22}, \delta_{23})$ . More generally, we can view the vector of deviations  $(\delta_{1n}, \delta_{2n}, \delta_{3n})$  as a representation of the datapoint  $z_n$  in the joint prediction space. In this sense, the matrix of predictions  $\{p_{nh}\}$  can be explained by the mean prediction 0.5 for each datapoint, together with two factors of variation (1, -1, 0) and (1, 0, -1) appropriately applied to each input. We next describe how to automatically extract such consistent high-level factors in an ensemble from the matrix of predictions.

#### J.2 PCA on Ensemble Predictions

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We propose to apply PCA to the  $H \times N$  matrix of residual predictions to obtain P principal components. Each principal component is a vector of size H that captures the orthogonal factors of variation in how ensemble members extrapolated from the training data. Given a set of weights  $w_1, \ldots, w_P$  over principal components, we can "reconstruct" a set of joint predictions as

$$p(x) = \bar{p}(x) + \begin{pmatrix} w_1 & \cdots & w_P \end{pmatrix} \begin{pmatrix} c_{11} & \cdots & c_{1H} \\ c_{21} & \cdots & c_{2H} \\ \vdots & \ddots & \vdots \\ c_{P1} & \cdots & c_{PH} \end{pmatrix} \begin{pmatrix} p_1(x) - \bar{p}(x) \\ p_2(x) - \bar{p}(x) \\ \vdots \\ p_H(x) - \bar{p}(x) \end{pmatrix},$$
(9)

976 where we denote the mean prediction as  $\bar{p}(x) = \frac{1}{H} \sum_{h} p_{nh}$  and the *P* principal components as  $C \in \mathbb{R}^{P \times H}$ .

We highlight two known interpretations of PCA that have interesting implications for our goal of summarizing ensemble predictions:

980 **Maximum mutual information / variance after projection.** PCA finds the linear projection  $y = w^{\top}x$  with unit vector w981 that achieves maximum mutual information I(x; y), or equivalently, maximum variance Var(y). Each principal component 982 finds the linear combination of ensemble members that preserves the most information about the set of joint ensemble 983 predictions. This is closely related to the disagreement term in Bayesian active learning (Houlsby et al., 2011).

Factor model. The principal components are maximum likelihood parameters under a linear Gaussian factor model of the data (Tipping & Bishop, 1999). Indeed, we can view our principal components as orthogonal modifications to the mean prediction  $\bar{p}(x)$ . The distribution of ensemble members is closely approximated by "reconstructed predictions" (9), where  $z_{1:P} \sim \mathcal{N}(0, I^P)$ . We can view each principal component as a consistent high-level direction of functional variation in which the training data provided insufficient information.

# 990 K PERSONA Dataset Details

Below, we list the personas used in our PERSONA (Castricato et al., 2024) experiments. The dataset includes 1000 personas in total, each with 200 preference pairs. We subsampled 10 personas from the original dataset of 1000, ensuring a diverse set of backgrounds, ages, and lifestyles.

995 Persona 1. Age: 1. Sex: Male. Race: White alone. Ancestry: Irish. Household language: English only. Education: 996 Not applicable. Employment status: Not applicable. Class of worker: Not applicable. Industry category: Not applicable. 997 Occupation category: Not applicable. Detailed job description: Not applicable. Income: Not applicable. Marital status: 998 Too young to be married. Household type: Cohabiting couple household with children of the householder less than 18. 999 Family presence and age: With related children under 5 years only. Place of birth: Missouri/MO. Citizenship: Born in 1000 the United States. Veteran status: Not applicable. Disability: None. Health insurance: With health insurance coverage. 1001 Fertility: Not applicable. Hearing difficulty: None. Vision difficulty: None. Cognitive difficulty: None. Ability to speak 1002 english: Not applicable. Big five scores: Openness: High, Conscientiousness: High, Extraversion: Low, Agreeableness: 1003 Extremely High, Neuroticism: Extremely Low. Defining quirks: Loves to play with his food. Mannerisms: Waves hands 1004 when excited. Personal time: Spends most of his time playing, sleeping, and learning to walk. Lifestyle: Lives a carefree 1005 and playful lifestyle. Ideology: Not applicable. Political views: Not applicable. Religion: Other Christian.

1006 Persona 2. Age: 11. Sex: Male. Race: White alone. Ancestry: Irish. Household language: English only. Education: Grade 1007 4. Employment status: Unemployed. Class of worker: Not applicable. Industry category: Not applicable. occupation 1008 category: Not applicable Detailed job description: Student. Income: 0. Marital status: Never married or under 15 years 1009 old. Household type: Cohabiting couple household with children of the householder less than 18. Family presence and age: With related children 5 to 17 years only. Place of birth: Louisiana/LA. Citizenship: Born in the United States. Veteran status: Not applicable. Disability: None. Health insurance: With health insurance coverage. Big five scores: Openness: 1012 Low, Conscientiousness: Low, Extraversion: High, Agreeableness: High, Neuroticism: Average. defining quirks: Loves to draw and create stories Mannerisms: Often seen doodling or daydreaming. Personal time: Spends free time drawing or 1014 playing video games. Lifestyle: Active and playful, enjoys school and spending time with friends. Ideology: Undeveloped. 1015 Political views: Undeveloped. Religion: Religiously Unaffiliated. 1016

Persona 3. Age: 19. Sex: Male. Race: Asian Indian alone. Ancestry: Indian. Household language: Hindi. Education: 1 or
more years of college credit, no degree. Employment status: Not in labor force. Class of worker: Not Applicable. Industry
category: Not Applicable. Occupation category: Not Applicable. Detailed job description: Not Applicable. Income: 60000.0. Marital status: Never married or under 15 years old. Household type: Living with parents. Family presence and
age: Living with two parents. Place of birth: India. Citizenship: Not a U.S. citizen. Veteran status: Non-Veteran. Disability:
None. Health insurance: With health insurance coverage. Big five scores: Openness: Average, Conscientiousness: High,
Extraversion: Extremely Low, Agreeableness: Extremely High, Neuroticism: Extremely Low. defining quirks: Passionate
about music Mannerisms: Expressive hand gestures when speaking. Personal time: Practicing music or studying. Lifestyle:
Student and Music Enthusiast. Ideology: Liberal. Political views: Liberal. Religion: Other Christian.

Persona 4. Age: 29. Sex: Female. Race: Laotian alone. Ancestry: Laotian. Household language: Asian and Pacific Island languages. Education: Some college, but less than 1 year. Employment status: Armed forces, at work. Class of worker: Federal government employee. Industry category: MIL-U.S. Navy. Occupation category: MIL-Military Enlisted Tactical Operations And Air/Weapons Specialists And Crew Members. Detailed job description: Maintains and operates tactical weapons systems. Income: 81000.0. Marital status: Married. Household type: Married couple household with children of the householder less than 18. Family presence and age: With related children 5 to 17 years only. Place of birth: California/CA. Citizenship: Born in the United States. Veteran status: Now on active duty. Disability: None. Health insurance: With health insurance coverage. Big five scores: Openness: Average, Conscientiousness: High, Extraversion: Average, Agreeableness: High, Neuroticism: Average. Defining quirks: Collects military memorabilia. Mannerisms: Frequently uses military jargon. Personal time: Spends time with family and collecting military memorabilia. Lifestyle: Disciplined and active. Ideology: Conservative. Political views: Republican. Religion: Protestant.

Persona 5. Age: 36. Sex: Female. Race: Some Other Race alone. Ancestry: Hispanic. Household language: English.
Education: Regular high school diploma. Employment status: Civilian employed, at work. Class of worker: Employee of
a private for-profit company or business, or of an individual, for wages, salary, or commissions. Industry category: FINInsurance Carriers. Occupation category: OFF-Insurance Claims And Policy Processing Clerks. Detailed job description:
Processes insurance claims and policies. Income: 182000.0. Marital status: Married. Household type: Married couple
household with children of the householder less than 18. Family presence and age: With related children under 5 years

only. Place of birth: New Mexico/NM. Citizenship: Born in the United States. veteran status: Non-Veteran Disability:
None. Health insurance: With health insurance coverage. Big five scores: Openness: Extremely Low, Conscientiousness:
Extremely High, Extraversion: Extremely High, Agreeableness: High, Neuroticism: Average. Defining quirks: Enjoys
bird-watching. Mannerisms: Often taps foot when thinking. Personal time: Spends free time with family or in nature.
Lifestyle: Active and family-oriented. Ideology: Conservative. Political views: Republican. Religion: Other Christian.

Persona 6. Age: 44. Sex: Female. Race: Black or African American alone. Ancestry: Haitian. household language: Other Indo-European languages education: Associate's degree Employment status: Civilian employed, at work. Class 1052 of worker: Employee of a private not-for-profit, tax-exempt, or charitable organization. Industry category: FIN-Banking And Related Activities. Occupation category: OFF-Tellers. Detailed job description: Handles customer transactions at the 1054 bank, including deposits, withdrawals, and loan payments. Income: 40000.0. Marital status: Separated. Household type: Female householder, no spouse/partner present, with children of the householder less than 18. Family presence and age: 1056 With related children 5 to 17 years only. Place of birth: Haiti. Citizenship: Not a U.S. citizen. Veteran status: Non-Veteran. Disability: None. Health insurance: With health insurance coverage. Big five scores: Openness: High, Conscientiousness: Extremely Low, Extraversion: Average, Agreeableness: Average, Neuroticism: Extremely Low. Defining quirks: Loves 1059 to cook Haitian cuisine. Mannerisms: Often taps her foot when stressed. Personal time: Taking care of her children, 1060 Pursuing further education. Lifestyle: Busy, Family-oriented. Ideology: Egalitarian. Political views: Democrat. Religion: 1061 Protestant. 1062

Persona 7. Age: 52. Sex: Female. Race: Korean alone. Ancestry: Korean. Household language: Asian and Pacific Island 1063 1064 languages. Education: Regular high school diploma. Employment status: Civilian employed, at work. Class of worker: State government employee. Industry category: ENT-Restaurants And Other Food Services. Occupation category: EAT-1065 1066 First-Line Supervisors Of Food Preparation And Serving Workers. Detailed job description: Supervises food preparation 1067 and serving workers in a state government facility. Income: 133900.0. Marital status: Married. Household type: Married 1068 couple household, no children of the householder less than 18. Family presence and age: No related children. Place of birth: Korea. Citizenship: U.S. citizen by naturalization. Veteran status: Non-Veteran. Disability: None. Health insurance: 1069 With health insurance coverage. big five scores: Openness: Average, Conscientiousness: Extremely High, Extraversion: Extremely Low, Agreeableness: Extremely Low, Neuroticism: Average defining quirks: Deep love for literature and reading Mannerisms: Constantly adjusts her glasses. Personal time: Spends free time reading or engaging in community 1072 activism. Lifestyle: Quiet and community-oriented. Ideology: Liberal. Political views: Democratic. Religion: Protestant.

Persona 8. Age: 58. Sex: Male. Race: White. Ancestry: Scottish. Household language: English. Education: Bachelor's Degree. Employment status: Employed. Class of worker: Private. industry category: Investigation And Security Services Occupation category: Sales Manager. Detailed job description: Oversees sales teams, sets sales goals, and develops strategies to achieve these goals. Income: 198200. Marital status: Married. Household type: Married couple household, no children under 18. Family presence and age: No related children. Place of birth: Florida. Citizenship: US Citizen. veteran status: Non-Veteran Disability: With a disability. Health insurance: With health insurance coverage. Big five scores: Openness: High, Conscientiousness: Extremely High, Extraversion: Average, Agreeableness: Average, Neuroticism: Average. Defining quirks: Keen interest in security technology and crime novels. mannerisms: Constantly checks his surroundings Personal time: Researching the latest security technologies or enjoying a round of golf. Lifestyle: Active and health-conscious. Ideology: Conservative. Political views: Republican. Religion: Catholic.

Persona 9. Age: 65. Sex: Female. Race: White alone. Ancestry: Italian. Household language: Other Indo-European languages. Education: Master's degree. Employment status: Civilian employed, at work. Class of worker: Self-employed 1087 in own incorporated business, professional practice or farm. Industry category: ENT-Traveler Accommodation. Occupation category: FIN-Accountants And Auditors. Detailed job description: Manages financial records and tax data for 1088 1089 her own travel accommodation business. Income: 188600.0. Marital status: Married. Household type: Married couple household, no children of the householder less than 18. Family presence and age: No related children. Place of birth: 1090 Delaware/DE. Citizenship: Born in the United States. Veteran status: Non-veteran. Disability: None. Health insurance: 1091 1092 With health insurance coverage, ability to speak english: Well. Big five scores: Openness: Average, Conscientiousness: 1093 Low, Extraversion: Low, Agreeableness: Average, Neuroticism: Extremely High. Defining quirks: Has an extensive col-1094 lection of vintage travel posters. Mannerisms: Tends to use Italian phrases in conversation. Personal time: Spends her free time exploring new places, trying new cuisines, and learning about different cultures. Lifestyle: Leads a busy lifestyle 1095 managing her business, but always finds time for her passion for travel and culture. Ideology: Believes in the importance 1096 1097 of understanding and appreciating different cultures. Political views: Liberal. Religion: Protestant. 1098

Persona 10. Age: 75. Sex: Female. Race: White alone. ancestry: Scottish Household language: English only. Education: Professional degree beyond a bachelor's degree. Employment status: Not in labor force. Class of worker: Retired. Industry category: Healthcare. Occupation category: Doctor. Detailed job description: Retired pediatrician. Income: 98000.0. Marital status: Never married. Household type: Female householder, no spouse/partner present, living alone. Family presence and age: No family. Place of birth: Massachusetts/MA. citizenship: Born in the United States veteran status: Non-Veteran Disability: None. Health insurance: With health insurance coverage. Big five scores: Openness: Average, Conscientiousness: Average, Extraversion: High, Agreeableness: Extremely High, Neuroticism: Average. Defining quirks: Enjoys cooking traditional Scottish meals. Mannerisms: Often hums traditional Scottish tunes. Personal time: Spends free time volunteering at the local church and community center. Lifestyle: Active but relaxed, with a focus on maintaining health and staying involved in the community. Ideology: Conservative. Political views: Republican. Religion: Catholic. 



Figure 8: Additional visualizations for the toy conflicting classification example. Increasing the scale hyperparameter results produces heads with sharper decision boundaries.



Figure 9: Detailed results for the personalizing preference reward models experiment in Figure 2. Target dataset accuracy (y-axis) after observing different numbers of adaptation samples (x-axis). The dashed line represents the performance of the pretrained reward model.