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PROBABLY APPROXIMATELY CORRECT LABELS

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ABSTRACT

Obtaining high-quality labeled datasets is often costly, requiring either human annotation or expensive experiments. In theory, powerful pre-trained AI models provide an opportunity to automatically label datasets and save costs. Unfortunately, these models come with no guarantees on their accuracy, making wholesale replacement of manual labeling impractical. In this work, we propose a method for leveraging pre-trained AI models to curate cost-effective and high-quality datasets. In particular, our approach results in *probably approximately correct labels*: with high probability, the overall labeling error is small. Our method is nonasymptotically valid under minimal assumptions on the dataset or the AI model being studied, and thus enables rigorous yet efficient dataset curation using modern AI models. We demonstrate the benefits of the methodology through text annotation with large language models, image labeling with pre-trained vision models, and protein folding analysis with AlphaFold.

1 INTRODUCTION

A key ingredient in any scientific pipeline is the availability of large amounts of high-quality *labeled* data. For example, social scientists rely on extensively-labeled datasets to understand human behavior (Salganik, 2017) and design policy interventions. Collecting high-quality labels for a given set of inputs is typically an arduous task that requires significant human expertise, costly large-scale experimentation, or expensive simulations. As such, researchers often outsource label collection to a third party “data provider”—this might be an annotation platform for labeling images, a wet lab for running scientific experiments, or a survey platform for collecting responses from a target population of individuals.

For data providers, the high cost of collecting high-quality labels combined with the rising performance of AI models suggests an enticing prospect: using AI *predictions* in place of manually-collected labels. Indeed, recent works have demonstrated AI models’ ability to predict protein structures (Jumper et al., 2021), to evaluate language model responses (Zheng et al., 2023), and even to simulate human experimental subjects (Argyle et al., 2023). These advances highlight the potential for AI to streamline data annotation, and to produce high-quality labels at a fraction of the cost.

The problem with such an approach is that AI models are not always accurate, and come with no guarantees on how well they will label a given dataset. This makes it untenable to use AI-predicted labels as a direct substitute for expert labels, particularly in settings where label quality is critical. For instance, if the downstream goal is to draw conclusions that inform policy decisions, we should not blindly treat AI predictions of human behavior as if they were experimentally collected data.

Motivated by this state of affairs, in this paper we ask:

Can we leverage powerful AI models to label data, while still guaranteeing quality?

We answer this question in the affirmative, and provide a method—which we call *probably approximately correct* (PAC) labeling—that automatically combines cheap, non-expert labels (whether AI predictions, crowd-sourced labels, or simple heuristics) with expensive, expert labels to produce a labeled dataset with small error. PAC labeling yields guarantees similar in flavor to that of its namesake in probably approximately correct (PAC) learning (Valiant, 1984): given user-specified constants $\epsilon, \alpha > 0$, our procedure results in a labeled dataset with error at most ϵ , with probability at least $1 - \alpha$. This guarantee is *nonasymptotic* under minimal assumptions on the dataset or the predicted labels being used.

054 1.1 CONTRIBUTIONS
055

056 We give a brief overview of our contributions, beginning with the problem setup. Given an unlabeled
057 dataset $X_1, \dots, X_n \in \mathcal{X}$, with unknown expert labels Y_1, \dots, Y_n , our goal is to return a labeled
058 dataset $(X_1, \tilde{Y}_1), \dots, (X_n, \tilde{Y}_n)$, such that we incur only a small amount of labeling errors:

$$059 \quad 060 \quad 061 \quad 062 \quad \frac{1}{n} \sum_{i=1}^n \ell(Y_i, \tilde{Y}_i) \leq \epsilon, \text{ with probability } 1 - \alpha. \quad (1)$$

063 Here, α and ϵ are user-chosen error parameters and ℓ is a relevant error metric. For example, if
064 we want categorical labels to be accurate, we can choose the 0-1 loss: $\ell(Y_i, \tilde{Y}_i) = \mathbf{1}\{Y_i \neq \tilde{Y}_i\}$.
065 The guarantee (1) then requires that at most an ϵ -fraction of the dataset is mislabeled, with high
066 probability. In regression problems, one might choose the squared loss, $\ell(Y_i, \tilde{Y}_i) = (Y_i - \tilde{Y}_i)^2$. We
067 call \tilde{Y}_i that satisfy the criterion (1) *probably approximately correct* (PAC) labels. To avoid strong
068 assumptions, we treat the data as *fixed*; probabilities are taken only over the labeling algorithm.

069 To produce the label \tilde{Y}_i , we are allowed to query an expert for Y_i , which is costly, or instead use a
070 cheap AI prediction $\hat{Y}_i = f(X_i)$, where f is an AI model. The prediction \hat{Y}_i can depend on any
071 feature information available for point i , as well as any source of randomness internal to f . We will
072 consider two settings: a basic setting with a single AI model f , and a more complex setting that
073 assumes access to k different models f_1, \dots, f_k .

074 Of course, we can trivially achieve (1) by collecting expert labels for all n data points. The goal
075 is to achieve the criterion while minimizing the cost of the labeling. We will consider two ways
076 of measuring the cost. The basic one is to simply count the number of collected expert labels; the
077 AI-predicted labels are assumed to essentially come at no cost. The second way of measuring the
078 cost takes into account the costs c_1, \dots, c_k of querying the k models, as well as the cost of an expert
079 label c_{expert} . When c_{expert} is much larger than c_1, \dots, c_k , the second setting reduces to the first.

080 Our main contribution is a method for producing PAC labels which, as we will show through a
081 series of examples across data modalities and AI models, allow for significant saves in labeling cost.
082 The key feature that enables a cost reduction is access to a measure of model uncertainty, which
083 allows focusing the expert budget on instances where the model is most uncertain. Crucially, the
084 nonasymptotic validity of PAC labeling does *not* depend on the quality of the uncertainties; more
085 useful measures lead to larger saves in cost. We provide refinements of the method that additionally
086 learn to calibrate the uncertainty scores to make the saves in cost even more pronounced.

087 1.2 RELATED WORK
088

089 **Adaptive dataset labeling and curation.** Our work most closely relates to the literature on efficient
090 dataset labeling from possibly noisy labels. A distinguishing feature of our work is that we construct
091 *provably accurate* labels with nonasymptotic guarantees, under no assumptions on the noisy labels.
092 In contrast, much of existing work makes strong parametric or distributional assumptions—for ex-
093 ample, model errors following a truncated power-law (Qiu et al., 2020) or a low-noise (Wang et al.,
094 2021) distribution, the data following a well-specified parametric family (Ratner et al., 2016), or a
095 class-conditional noise process (Northcutt et al., 2021). Many works lack formal accuracy guar-
096antees (Zhu & Ghahramani, 2002; Iscen et al., 2019; Bernhardt et al., 2022; Li et al., 2023; Xie et al.,
097 2020). Since we do not place distributional assumptions on the data but instead consider it fixed,
098 our work particularly relates to the labeling problem known as transductive learning (Vapnik, 1998;
099 Joachims, 2003). A key feature of our work is that we leverage pre-trained AI models, such as off-
100 the-shelf language or vision models, and make no complexity assumptions on the expert labeling
101 mechanism. An emerging line of work studies human-AI collaborative approaches to dataset cura-
102 tion (Li et al., 2023; Yuan et al., 2021; Liu et al., 2022; Kay et al., 2025). Our work is motivated by
103 similar problems, with a focus on ensuring statistical validity. Importantly, many of the above works
104 use uncertainty to decide which labels to collect (Bernhardt et al., 2022; Li et al., 2023; Kay et al.,
105 2025). Our work similarly relies on uncertainty; in fact, our procedure can be applied as a wrapper
106 around *any* uncertainty score to provide a statistically valid labeling. For example, the CoAnnotating
107 paradigm defines an uncertainty score and proposes annotating the top k most uncertain points with
108 human annotations and the rest with AI annotations, for some user-chosen k . Our procedure can be
109 applied to select k in a data-driven manner, so that the final labeling is $(1 - \epsilon)$ -accurate with high

108 probability. A similar observation applies to the CODA framework (Kay et al., 2025): our work can
 109 be applied as a wrapper around the expected information gain (EIG) used in CODA. More distant
 110 but related is a vast line of work studying different strategies for reliable aggregation of multiple
 111 noisy labels (Karger et al., 2014; Cheng et al., 2022; Dawid & Skene, 1979; Whitehill et al., 2009;
 112 Zhang & Chaudhuri, 2015; Yan et al., 2010; Welinder et al., 2010; Sheng et al., 2008; Yan et al.,
 113 2011).

114 **Distribution-free uncertainty quantification.** At a technical level, our procedure resembles the
 115 construction of risk-controlling prediction sets (Bates et al., 2021) and performing risk-limiting au-
 116 ditis (Waudby-Smith et al., 2021; Shekhar et al., 2023). Like the former, our procedure bounds a
 117 monotone loss function by tuning a one-dimensional threshold, though not for the purpose of pre-
 118 dictive inference. Similarly to the latter, our procedure aims to collect sufficient expert labels so as
 119 to meet a pre-specified quality guarantee. Like all these methods, PAC labeling satisfies *nonasym-
 120 ptotic, distribution-free* statistical guarantees. To achieve this, we build on betting-based confidence
 121 intervals (Waudby-Smith & Ramdas, 2024; Orabona & Jun, 2023). Our proposal relates in spirit to
 122 prediction-powered inference (Angelopoulos et al., 2023a; Zrnic & Candès, 2024a; Angelopoulos
 123 et al., 2023b) and related control-variate approaches (Zhou et al.; Egami et al., 2023), where the goal
 124 is to improve the power of statistical inferences given a small amount of expert-labeled data, a large
 125 amount of unlabeled data, and a good predictive model. We do not focus on statistical inference per
 126 se; rather, we construct an accurately labeled dataset that can be used for any downstream task.

127 **Active learning and inference.** The idea behind our method is to collect expert labels where the AI
 128 model is most uncertain; in that sense, our method relates to active learning (Settles, 2009; Lewis,
 129 1995; Beluch et al., 2018; Zhang & Chaudhuri, 2015) and active inference (Zrnic & Candès, 2024b;
 130 Gligorić et al., 2024). Notably, there is a line of work in active learning that considers costs (Settles
 131 et al., 2008; Donmez & Carbonell, 2008; Wang et al., 2016). Our goal is fundamentally different: it
 132 is neither fitting a predictive model nor statistical inference, but producing high-quality labeled data
 133 with a provable nonasymptotic guarantee under minimal assumptions. In general, this is neither
 134 necessary nor sufficient for active learning. A related problem is “learning to defer” (Madras et al.,
 135 2018), a framework for jointly optimizing a predictive model and decisions to defer to an expert.
 136 Learning to defer does not come with guarantees on the statistical validity of the final labels, and it
 137 does not assume black-box access to predicted labels; the learner trains a model from scratch.

2 PAC LABELING: CORE METHOD

140 We begin with the basic setting with one AI model that produces cheap labels. Thus, we have $\hat{Y}_i =$
 141 $f(X_i)$ for all data points. In addition, we assume access to scalar uncertainty scores U_1, \dots, U_n
 142 (typically scaled such that $U_i \in [0, 1]$) corresponding to the predictions $\hat{Y}_1, \dots, \hat{Y}_n$. We place no
 143 assumptions on the quality of U_i , however if lower U_i correspond to more accurate predictions \hat{Y}_i ,
 144 the procedure will achieve big gains. The PAC guarantee (1) holds no matter the quality of U_i .

145 The basic idea behind the procedure is to find an uncertainty threshold \hat{u} and label all data points
 146 with uncertainty that exceeds this threshold, $U_i \geq \hat{u}$. The more accurate the predictions \hat{Y}_i are, the
 147 higher this threshold will be. To explain how we set \hat{u} , we introduce some notation. Let $\ell^u(Y_i, \hat{Y}_i) =$
 148 $\ell(Y_i, \hat{Y}_i) \mathbf{1}\{U_i \leq u\}$ and $L^u = \frac{1}{n} \sum_{i=1}^n \ell^u(Y_i, \hat{Y}_i)$. Ideally, if we knew L^u for every u , we would
 149 choose the *oracle threshold*:

$$u^* = \min \{U_i : L^{U_i} > \epsilon\}.$$

150 In other words, if we label all points with $U_i \geq u^*$, meaning $\tilde{Y}_i = Y_i \mathbf{1}\{U_i \geq u^*\} + \hat{Y}_i \mathbf{1}\{U_i < u^*\}$,
 151 then we satisfy $\frac{1}{n} \sum_{i=1}^n \ell(Y_i, \tilde{Y}_i) \leq \epsilon$ with probability one. The issue is that we do not have access
 152 to Y_i , and thus we cannot compute L^{U_i} . To resolve this issue, we estimate an upper bound on L^{U_i} by
 153 initially collecting expert labels for a small subset of the data. We will soon explain such a strategy;
 154 for now assume that for every $\alpha \in (0, 1)$ and every u , we can obtain a valid upper confidence bound
 155 on L^u at level $1 - \alpha$, denoted $\hat{L}^u(\alpha)$: $\mathbb{P}(L^u \leq \hat{L}^u(\alpha)) \geq 1 - \alpha$. Note that we only require $\hat{L}^u(\alpha)$ to
 156 be valid one u at a time, not simultaneously. Our empirical approximation of the oracle threshold is
 157

$$\hat{u} = \min\{U_i : \hat{L}^{U_i}(\alpha) > \epsilon\}. \quad (2)$$

158 Therefore, we collect expert labels where our uncertainty is \hat{u} or higher: $\tilde{Y}_i = Y_i \mathbf{1}\{U_i \geq \hat{u}\} +$
 159 $\hat{Y}_i \mathbf{1}\{U_i < \hat{u}\}$. We argue that such labels are PAC labels.

162 **Theorem 1.** The labels $\tilde{Y}_i = Y_i \mathbf{1}\{U_i \geq \hat{u}\} + \hat{Y}_i \mathbf{1}\{U_i < \hat{u}\}$, with \hat{u} given by (2), are PAC labels (1).
 163

164 Interestingly, notice that the proof only requires $\hat{L}^{U_i}(\alpha)$ to be valid *individually*, even though we
 165 form n confidence bounds. This is a consequence of the monotonicity of L^u in u , similar in spirit to
 166 how monotonicity enables the Dvoretzky–Kiefer–Wolfowitz inequality (Dvoretzky et al., 1956) and
 167 risk-controlling prediction sets (Bates et al., 2021) to be free of multiplicity corrections.

168 It remains to provide a method to compute $\hat{L}^{U_i}(\alpha)$. Given a hyperparameter m , we collect m draws
 169 $\{i_1, \dots, i_m\}$ independently as $i_j \sim \text{Unif}([n])$. Then, for all $j \in [m]$, we sample $\xi_{i_j} \sim \text{Bern}(\pi_{i_j})$,
 170 where (π_1, \dots, π_n) are arbitrary sampling weights, and collect \tilde{Y}_{i_j} if $\xi_{i_j} = 1$. This results in a
 171 dataset of m i.i.d. variables $\{\ell(Y_{i_j}, \hat{Y}_{i_j}) \frac{\xi_{i_j}}{\pi_{i_j}}\}_{j=1}^m$; therefore, we can estimate $\hat{L}^u(\alpha)$ as:
 172

$$\hat{L}^u(\alpha) = \text{meanUB}(\{\ell(Y_{i_j}, \hat{Y}_{i_j}) \xi_{i_j} / \pi_{i_j} \mathbf{1}\{U_{i_j} \leq u\}\}_{j=1}^m; \alpha).$$

173 Here, $\text{meanUB}(\cdot; \alpha)$ is any method for computing a valid upper bound at level $1 - \alpha$ on the mean
 174 from an i.i.d. sample. Indeed, the samples $\ell(Y_{i_j}, \hat{Y}_{i_j}) \frac{\xi_{i_j}}{\pi_{i_j}} \mathbf{1}\{U_{i_j} \leq u\}$ are i.i.d. with mean L^u , since
 175 $\mathbb{E}[\xi_{i_j} / \pi_{i_j} | i_j] = 1$. The motivation for allowing adaptive sampling weights π_i is to allow forming
 176 a tighter confidence bound through a careful choice of the weights, although even uniform weights
 177 $\pi_1 = \dots = \pi_n = p \in (0, 1)$ are a reasonable choice in practice.

178 There are many possible choices for $\text{meanUB}(\cdot; \alpha)$: it can be a nonasymptotic procedure such
 179 as the betting-based confidence intervals (Waudby-Smith & Ramdas, 2024), or (if one is satisfied
 180 with asymptotic guarantees) simply a confidence bound based on the central limit theorem:
 181 $\text{meanUB}(\{Z_j\}_{j=1}^m; \alpha) = \hat{\mu}_Z + z_{1-\alpha} \frac{\hat{\sigma}_Z}{\sqrt{m}}$, where $\hat{\mu}_Z$ and $\hat{\sigma}_Z$ are the empirical mean and standard
 182 deviation of $\{Z_j\}_{j=1}^m$, respectively, and $z_{1-\alpha}$ is the $(1 - \alpha)$ -quantile of the standard normal distribution.
 183 In our experiments, we will primarily focus on procedures with nonasymptotic validity.
 184

185 We summarize the overall procedure in Algorithm 1 and its guarantee in Corollary 1.
 186

187 **Corollary 1.** For any valid mean upper bound subroutine meanUB , Algorithm 1 outputs PAC labels.
 188

189 **Uncertainty calibration.** The utility of PAC labeling crucially depends on the quality of the uncertainty
 190 scores. However, some data points X_i might have more accurate uncertainties than others.
 191 For example, suppose we can partition the X_i 's into two groups: on one, the model is consistently
 192 overconfident, and on the other, the model is consistently underconfident. Then, PAC labeling will
 193 overcollect expert labels for the data points in the second group. In the extreme case, imagine the
 194 model is incorrect on data points from the first group but produces low uncertainties, and is correct
 195 on data points from the second group but produces high uncertainties. Then, all expert labels for the
 196 second group will be collected. This is clearly wasteful, especially if the second group is large.

197 We propose uncertainty calibration to mitigate this issue. A natural way to calibrate uncertainties
 198 arises when there is a collection \mathcal{C} of (possibly overlapping) clusters in the data. These clusters could
 199 be implied by externally given features (e.g., demographics), or they could be discovered in a data-
 200 driven way. For the zero–one loss, we use the multicalibration algorithm from Hébert-Johnson et al.
 201 (2018), stated in Algorithm 2 in the Appendix for completeness, to learn the uncertainty adjustment
 202 for each cluster. In practice, we learn the adjustment by collecting expert labels for a small subset
 203 of size $m \ll n$ of the overall dataset and applying the correction to the remainder of the dataset.
 204

205 **Algorithm 1** Probably Approximately Correct Labeling

206 **Input:** unlabeled data X_1, \dots, X_n , predicted labels $\hat{Y}_1, \dots, \hat{Y}_n$, uncertainties U_1, \dots, U_n , labeling error ϵ ,
 207 error probability $\alpha \in (0, 1)$, sample size for estimation m , sampling weights π_1, \dots, π_n
 208 1: Sample $i_j \sim \text{Unif}([n])$ and $\xi_{i_j} \sim \text{Bern}(\pi_{i_j})$ independently for $j \in [m]$
 209 2: Collect \tilde{Y}_{i_j} if $\xi_{i_j} = 1$ for $j \in [m]$
 210 3: Compute confidence bound $\hat{L}^u(\alpha) = \text{meanUB} \left(\{\ell^u(Y_{i_j}, \hat{Y}_{i_j}) \frac{\xi_{i_j}}{\pi_{i_j}}\}_{j \in [m]}; \alpha \right)$, $\forall u \in \{U_i\}_{i=1}^n$
 211 4: Let $\hat{u} = \min\{U_i : \hat{L}^{U_i}(\alpha) > \epsilon\}$
 212 5: Collect true labels Y_i for points where $U_i \geq \hat{u}$
 213 6: Let $\tilde{Y}_i \leftarrow Y_i \mathbf{1}\{U_i \geq \hat{u}\} + \hat{Y}_i \mathbf{1}\{U_i < \hat{u}\}$ for all $i \in [n]$
 214 7: For all $\{i_j\}_{j \in [m]}$ s.t. $\xi_{i_j} = 1$, (possibly) update $\tilde{Y}_{i_j} \leftarrow Y_{i_j}$
 215 **Output:** labeled dataset $(X_1, \tilde{Y}_1), \dots, (X_n, \tilde{Y}_n)$

216

3 MULTI-MODEL LABELING VIA THE PAC ROUTER

217

218 In many cases, we have access to several different sources of non-expert predictions. For example,
219 we might have labels from several different AI models, or from (non-expert) human annotators of
220 varying skill levels. In such settings, we might hope to leverage the strengths of these different
221 predictors to reduce our overall labeling cost.

222 Concretely, consider a setting with k cheap labeling sources; for each data point i , each source
223 $j \in [k]$ provides a predicted label \hat{Y}_i^j and an uncertainty U_i^j . Our goal is to route each data point to
224 the most reliable source, minimizing the number of expert labels that we need to collect to retain the
225 guarantee (1). (We later move to a cost-sensitive setting.) Our high-level approach has two steps:

226

227 1. First, we will learn a *routing model* $w_\theta : \mathcal{X} \rightarrow \Delta^{k-1}$ that maps each data point to a distri-
228 bution over the k labeling sources. We use the routing model to find the best source j_i^* for
229 each data point i , to which we assign label $\hat{Y}_i = \hat{Y}_i^{j_i^*}$ and uncertainty $U_i = U_i^{j_i^*}$.
230 2. We then apply the PAC labeling procedure from Section 2 to the selected data points, using
231 the routed labels and uncertainties.

232 The main question is how to learn the routing model w_θ . Throughout, we will assume access to
233 a small, fully labeled *routing dataset* of size m , for which we observe $(X_i, Y_i, \{\hat{Y}_i^j, U_i^j\}_{j=1}^k)_{i=1}^m$,
234 which we can use to learn the routing model.

235 A natural first idea (but ultimately a suboptimal one) is to maximize the expected accuracy of the
236 routed labels—i.e., to solve $\arg \min_{\theta} \sum_{i=1}^m \sum_{j=1}^k w_{\theta,j}(X_i) \ell(Y_i, \hat{Y}_i^j)$, where $w_{\theta,j}(X_i)$ denotes the
237 j -th coordinate of $w_\theta(X_i)$. This router is suboptimal because it ignores models’ uncertainties and
238 our error tolerance ϵ . For example, consider the case where one labeling source has 100% accuracy
239 but is also highly uncertain. For the purposes of PAC labeling, this source is not helpful; indeed, it
240 will result in more expert labels being collected than if we had used the other sources. The router,
241 however, will be incentivized to route all points to this source to maximize expected accuracy.

242 Can we route points in a way that takes into account the ultimate cost of the labeling procedure? To
243 start, observe that the actual expected cost incurred by using a particular routing model w_θ is

244
$$\sum_{i=1}^m \sum_{j=1}^k w_{\theta,j}(X_i) \mathbf{1}\{U_i^j \geq \hat{u}\}, \quad (3)$$

245 where \hat{u} is the threshold set by the PAC labeling procedure. Ideally, we could minimize this quan-
246 tity directly, e.g., using gradient descent. There are two barriers to doing so: first, (3) is non-
247 differentiable due to the $\mathbf{1}\{\cdot\}$ term, and second, \hat{u} implicitly depends on the routing model w_θ itself.

248 To circumvent these issues, we first replace the indicator $\mathbf{1}\{U_i^j > \hat{u}\}$ with a sigmoid $\sigma(U_i^j - \hat{u})$. We
249 then consider the following differentiable relaxation of the PAC labeling scheme that allows us to
250 take gradients of our final objective with respect to the parameters of the routing model. Concretely,
251 we consider a labeling scheme based on a threshold \tilde{u} computed in the following way. We can
252 approximate the PAC labeling guarantee with a weaker guarantee of expected average error control,
253 then our procedure for finding \tilde{u} can be written as:

254
$$\tilde{u} \approx \min \left\{ u : \mathbb{E}_{X_i, Y_i, j \sim w_\theta(X_i)} [\ell(Y_i, \hat{Y}_i^j) \cdot \mathbf{1}\{U_i^j \leq u\}] > \epsilon \right\}, \quad (4)$$

255 where the expectation over X_i, Y_i denotes the empirical average over the (fixed) data points (X_i, Y_i) .
256 If we again replace the indicator $\mathbf{1}\{U_i^j \leq u\}$ with a sigmoid, then \tilde{u} is the solution to the equation:

257
$$\mathbb{E}_{X_i, Y_i} \left[\sum_{j=1}^k w_{\theta,j}(X_i) \cdot \ell(Y_i, \hat{Y}_i^j) \cdot \sigma(\tilde{u} - U_i^j) \right] = \epsilon. \quad (5)$$

258 By strict monotonicity of the sigmoid and positivity of the remaining terms, this solution is unique.
259 Therefore, we can write it as $\tilde{u}(\theta)$, and use the implicit function theorem to compute the gradient of
260 \tilde{u} with respect to θ . After a short derivation deferred to App. A.3, we get:

261
$$\nabla_\theta \tilde{u}(\theta) = - \frac{\mathbb{E}_{X_i, Y_i} \left[\sum_{j=1}^k \nabla_\theta w_{\theta,j}(X_i) \cdot \ell(Y_i, \hat{Y}_i^j) \cdot \sigma(u(\theta) - U_i^j) \right]}{\mathbb{E}_{X_i, Y_i} \left[\sum_{j=1}^k w_{\theta,j}(X_i) \cdot \ell(Y_i, \hat{Y}_i^j) \cdot \sigma(u(\theta) - U_i^j) \cdot (1 - \sigma(u(\theta) - U_i^j)) \right]}. \quad (6)$$

270 This gradient admits a more compact representation using a single expectation (see App. A.3). This
 271 suggests a natural algorithm for training w_θ : we compute the “smooth threshold” $\tilde{u}(\theta)$ by solving (5)
 272 (e.g., via binary search), and take a gradient step on the objective
 273

$$274 \sum_{i=1}^n \sum_{j=1}^k w_{\theta,j}(X_i) \cdot \ell(Y_i, \hat{Y}_i^j) \cdot \sigma(\tilde{u}(\theta) - U_i^j),$$

$$275$$

$$276$$

277 using the gradient (6) to backpropagate through the threshold computation; and finally we repeat the
 278 above two steps until convergence.

279 **Recalibrating uncertainties.** Even with a principled way to route data points to different models,
 280 in practice our performance will often be bottlenecked by the quality of the uncertainties U_i^j . In
 281 particular, if all of the models are uncalibrated on a given data point, then routing will not yield any
 282 benefit in terms of the number of expert labels collected. Furthermore, the uncertainty values do
 283 not reflect the fact that we have routed the data point to the source we expect to be most reliable.
 284 Motivated by these observations, we propose a procedure for simultaneously learning a routing
 285 model and a better uncertainty model. The main idea is exactly the same as before: we will define
 286 an uncertainty model $u_\gamma : \mathcal{X} \rightarrow [0, 1]$ that maps a data point to a new uncertainty value. To train the
 287 uncertainty model, we will use the same smoothed threshold procedure as before, noting now that
 288 the threshold $\tilde{u} = \tilde{u}(\theta, \gamma)$ depends on both the parameters of the routing model and the parameters of
 289 the uncertainty model. Accordingly, we perform gradient descent to solve the optimization problem

$$290 \min_{\theta, \gamma} \sum_{i=1}^m \sum_{j=1}^k w_{\theta,j}(X_i) \cdot \ell(Y_i, \hat{Y}_i^j) \cdot \sigma(\tilde{u}(\theta, \gamma) - u_\gamma(X_i)),$$

$$291$$

$$292$$

293 using implicit gradients $\nabla_\theta \tilde{u}(\theta, \gamma)$ and $\nabla_\gamma \tilde{u}(\theta, \gamma)$ derived using a similar logic as before (App. A.3).

294 **Cost-sensitive PAC router.** So far, we have treated the k cheap labeling sources as if they are free
 295 (or vanishingly cheap, compared to the cost of the expert labeler). In practice, however, we may
 296 want to take the cost of the labeling sources into account. For example, these different sources may
 297 represent running experiments with different numbers of crowd workers, or with public APIs that
 298 have different costs. Suppose each labeling source j has a per-label cost c_j , and that the cost of the
 299 expert labeler is c_{expert} . To incorporate costs, we use the same idea as the previous sections, aiming
 300 to directly optimize the expected cost incurred by the procedure. Our expected cost becomes

$$301 \sum_{i=1}^m \mathbb{E}_{j \sim w_\theta(X_i)} \left[c_j \cdot \mathbf{1}\{U_i^j < \hat{u}\} + c_{\text{expert}} \cdot \mathbf{1}\{U_i^j \geq \hat{u}\} \right],$$

$$302$$

$$303$$

304 where \hat{u} is the threshold computed using the main PAC labeling procedure. Just as in the previous
 305 sections: we approximate this threshold with a smoothed threshold \tilde{u} ; use implicit differentiation to
 306 derive the gradient of \tilde{u} with respect to the parameters of the routing and uncertainty models; replace
 307 indicators with sigmoids to get a fully differentiable objective; and perform gradient descent.

308 4 EXPERIMENTS

311 We evaluate PAC labeling on a series of real datasets, spanning natural language, computer vision,
 312 and proteomics. We repeat each experiment 1000 times and report the mean and standard deviation
 313 of the save in budget, i.e., the percentage of data points that are *not* expert labeled. We also report
 314 the $(1 - \alpha)$ -quantile of the empirical error $\frac{1}{n} \sum_{i=1}^n \ell(Y_i, \hat{Y}_i)$ (which is supposed to be upper bounded
 315 by ϵ). We plot the budget save against the realized error for 50 of the 1000 trials. We fix $\alpha = 0.05$.
 316 Except where otherwise noted, we use the betting algorithm of Waudby-Smith & Ramdas (2024) to
 317 compute mean upper bounds, with analogous results for the CLT-based upper bound in App. C.2.

318 We begin with PAC labeling experiments with a single AI model; we consider both problems with
 319 discrete and continuous labels. In this setting, we evaluate the benefits of uncertainty calibration.
 320 Then we study PAC labeling with multiple models, considering both the “costless” setting in which
 321 all AI predictions are treated as equally expensive, as well as the cost-sensitive setting that allows
 322 setting a different cost per AI model.

323 **PAC labeling with a single model.** We begin with the single-model case. In addition to PAC
 labeling, we consider two baselines. The first is the “naive” baseline, which collects expert labels

Dataset	Metric	Method			
		PAC labeling	Naive ($U_i \geq 0.1$)	Naive ($U_i \geq 0.05$)	AI only
Media bias	Budget save (%)	(13.79 \pm 3.38)%	17.76%	8.35%	—
	Error	4.10%	2.95%	1.10%	37.72%
Stance on global warming	Budget save (%)	(28.09 \pm 3.28)%	62.51%	25.10%	—
	Error	4.57%	10.13%	0.83%	24.79%
Misinformation	Budget save (%)	(18.12 \pm 4.93)%	50.44%	2.65%	—
	Error	3.80%	7.07%	0.10%	18.62%

Table 1: **PAC labeling text datasets with GPT-4o.** We set $\epsilon = 0.05$. PAC labeling meets the error criterion, the AI only baseline has a large error, and the fixed threshold baseline is sometimes valid and sometimes not. Even when it is valid, it can be conservative.

Dataset	Metric	Method			
		PAC labeling	Naive ($U_i \geq 0.1$)	Naive ($U_i \geq 0.05$)	AI only
ImageNet	Budget save (%)	(59.64 \pm 1.49)%	60.28%	52.79%	—
	Error	4.73%	3.15%	2.00%	21.69%
ImageNet v2	Budget save (%)	(39.07 \pm 2.67)%	46.05%	39.07%	—
	Error	4.74%	4.31%	2.62%	35.33%

Table 2: **PAC labeling image datasets with ResNet-152.** We set $\epsilon = 0.05$. PAC labeling and the fixed threshold baseline meet the error criterion and the AI only baseline has a large error. Even when it is valid, the fixed threshold baseline can be conservative.

for all points where the model’s uncertainty is above a fixed threshold, such as 10% or 5%. The second baseline is the method that only uses the AI labels, without using any expert labels.

Discrete labels. First we study the problem of collecting discrete labels; thus, we use the zero-one loss, $\ell(Y_i, \hat{Y}_i) = \mathbf{1}\{Y_i \neq \hat{Y}_i\}$. We consider several text annotation tasks from computational social science: labeling whether a text contains misinformation ($Y_i \in \{\text{misinfo, real}\}$) (Gabriel et al., 2022), labeling whether media headlines agree that global warming is a serious concern ($Y_i \in \{\text{agree, neutral, disagree}\}$) (Luo et al., 2020), and labeling of political bias of media articles ($Y_i \in \{\text{left, center, right}\}$) (Baly et al., 2020). We use predicted labels \hat{Y}_i from GPT-4o, collected by Gligorić et al. (2024). For the uncertainties U_i , we use GPT’s verbalized confidence scores; that is, we prompt the model to state its confidence in the answer. Additionally, we consider image labeling on ImageNet and ImageNet v2. We use the ResNet-152 to obtain \hat{Y}_i , and set $U_i = 1 - p_{\max}(X_i)$, where $p_{\max}(X_i)$ is the maximum softmax output given image X_i .

We summarize the results in Table 1, Table 2, and Figure 1. Using a fixed uncertainty threshold such as 5% or 10% results in highly variable results across datasets; sometimes the naive baseline is valid, sometimes it is not, and when it is valid often it is conservative. The approach of using AI labels alone achieves error that is far above the nominal. PAC labeling achieves error that fluctuates tightly around ϵ , and the budget saves range between 14% and 60% depending on the difficulty of the labeling. We include plots analogous to those in Figure 1 for the remaining datasets in App. C.1.

Continuous labels. By choosing the appropriate loss, PAC labeling applies to continuous labels. The first task we consider is sentiment analysis (Socher et al., 2013). The goal is to provide a real-valued sentiment score $Y_i \in [0, 1]$ of a phrase, higher indicating more a positive sentiment. We use the squared loss, $\ell(Y_i, \hat{Y}_i) = (Y_i - \hat{Y}_i)^2$. We use GPT-4o to collect predicted labels \hat{Y}_i and uncertainties U_i : we prompt GPT to predict an interval $[a_i, b_i]$ for the label Y_i , set $\hat{Y}_i = \frac{a_i + b_i}{2}$ and use the length of the interval as the uncertainty score, $U_i = b_i - a_i$. The second task is protein structure prediction. Here, Y_i are experimentally derived structures and \hat{Y}_i are AlphaFold predictions (Jumper et al., 2021). We use the mean squared deviation (MSD), the standard measure of protein structure quality, as the loss ℓ . For context, two experimental structures for the *same* protein have a gap of around 0.36 in terms of MSD. For the uncertainties U_i , we use the average predicted local distance difference test (pLDDT), AlphaFold’s internal measure of local confidence. We use the CLT upper bound as the mean upper bound subroutine in the algorithm.

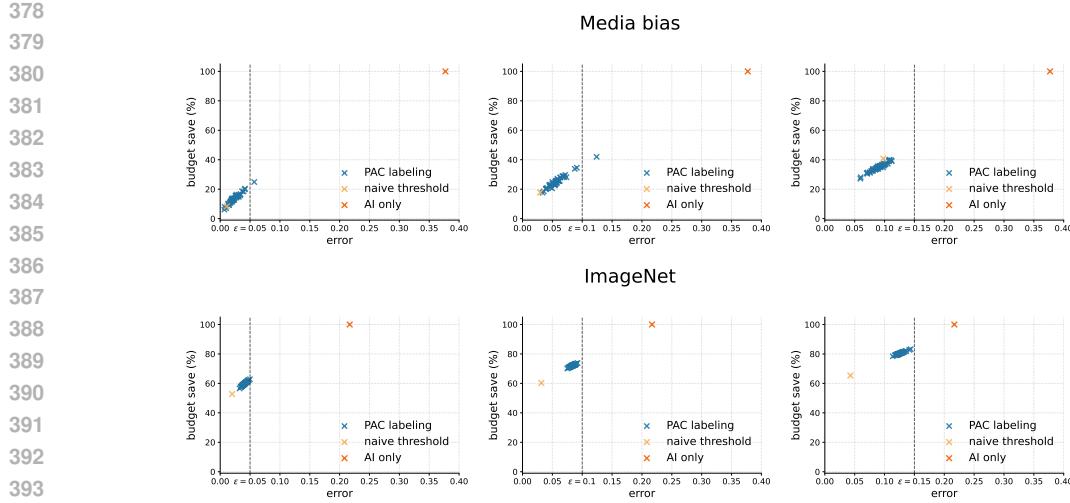


Figure 1: **PAC labeling for discrete labels.** Realized error and save in budget for PAC labeling, the naive thresholding baseline, and the AI only baseline. Each row and column correspond to a different dataset and value of ϵ (denoted by vertical dashed line), respectively. For the naive thresholding baseline, we collect expert labels for all points with $U_i \geq \epsilon$.

Dataset	Metric	Method			
		PAC ($\epsilon = 0.005$)	PAC ($\epsilon = 0.01$)	PAC ($\epsilon = 0.015$)	AI only
Sentiment analysis	Budget save (%)	(16.03 \pm 2.49)%	(33.25 \pm 3.47)%	(50.86 \pm 3.93)%	—
	Error	0.004	0.009	0.013	0.021
Protein folding	PAC ($\epsilon = 0.36$)	PAC ($\epsilon = 0.64$)	PAC ($\epsilon = 1.0$)	AI only	
	Budget save (%)	(19.93 \pm 1.54)%	(26.47 \pm 3.37)%	(33.99 \pm 3.76)%	—
	Error	0.367	0.608	0.944	3.58

Table 3: **PAC labeling for continuous labels.** PAC labeling (approximately) meets the error criterion, while the AI only baseline has a large error.

Dataset	Metric	Method	
		PAC (before calibration)	PAC (after calibration)
Media bias	Budget save (%)	(13.68 \pm 3.19)%	(16.72 \pm 2.81)%
	Error	4.10%	4.22%

Table 4: **Uncertainty calibration.** We set $\epsilon = 0.05$. PAC labeling with calibrated uncertainties (right) leads to higher saves than PAC labeling without calibration (left).

We summarize the results in Table 3 and Figure 2. For all ϵ , PAC labeling tightly controls error while saving a nontrivial fraction of expert labels; the AI-only baseline does not meet the error criterion.

Uncertainty calibration. Calibrating uncertainties is a simple way to improve the performance of PAC labeling. In Table 4, we show the results of PAC labeling with GPT-4o on the media bias dataset (Baly et al., 2020), with a very simple calibration procedure: we use GPT-4o to cluster the articles into five clusters based on how conservative/liberal their source (e.g., CNN, Fox News, NYT, etc.) is, and we treat each article’s cluster assignment as a group label G_i . We iterate through each group and uncertainty bin and additively adjust the uncertainties to match the average correctness using a small calibration set, as described in Section 2. Even in this simple setting (where the group labels are disjoint and derived only from the article source), calibration leads to a noticeable gain.

PAC labeling with multiple models. Next, we consider the multi-model case. We revisit the problem of annotating the political bias of media articles (Baly et al., 2020). In addition to GPT-4o predictions and confidences, we also collect predictions and confidences from Claude 3.7 Sonnet. We train a PAC router to route the articles between the two language models, while simultaneously training an uncertainty model, as described in Section 3.

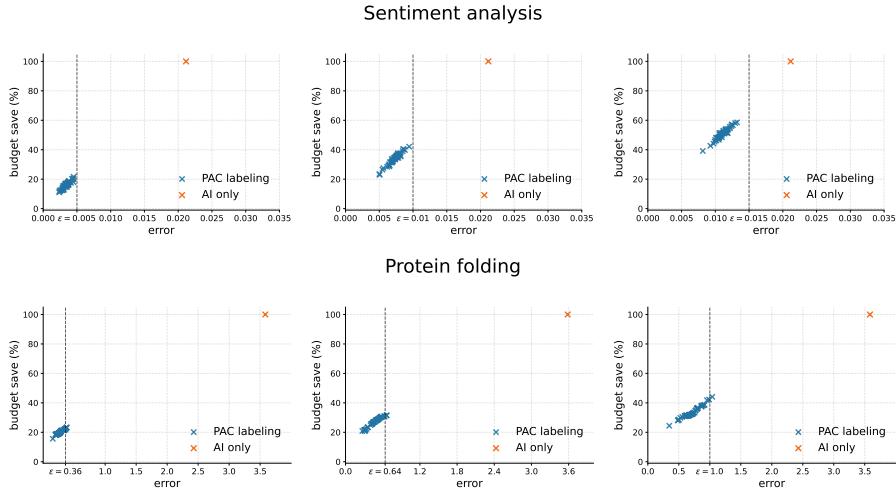


Figure 2: **PAC labeling for continuous labels.** Realized error and save in budget for PAC labeling and the AI only baseline. Each row and column correspond to a different dataset and value of ϵ (denoted by vertical dashed line), respectively.

Dataset	Metric	Method		
		PAC labeling (GPT-4o)	PAC labeling (Claude Sonnet)	PAC router
Media bias	Budget save (%)	$(13.79 \pm 3.38)\%$	$(8.41 \pm 3.01)\%$	$(41.61 \pm 1.50)\%$
	Error	4.10%	4.00%	4.61%
	Save in cost	$(188.66 \pm 41.15)\%$	$(131.36 \pm 49.20)\%$	$(482.04 \pm 114.73)\%$
	Error	4.06%	3.58%	3.61%

Table 5: **PAC router for language models.** We set $\epsilon = 0.05$. The PAC router significantly improves the budget save (top) and save in cost (bottom) compared to PAC labeling with individual models.

Costless predictions. First we consider the setting of costless predictions, aiming only to minimize the number of collected expert labels. See Figure 3 (top) and Table 5 (top) for the results. GPT and Claude alone yield a 14% and 8% budget save, respectively, while by routing between the two saves about 42% of the expert label cost. To give intuition for how this gain is achieved, in Appendix Figure 4 we plot the loss $L^u = \frac{1}{n} \sum_{i=1}^n \ell^u(Y_i, \hat{Y}_i)$ resulting from collecting labels at uncertainties greater than or equal to u , as a function of u . We observe that the router produces a curve L^u that strictly dominates the loss curves of the individual models. This means that for any uncertainty threshold, the resulting labeling achieves a strictly smaller error than with a single model.

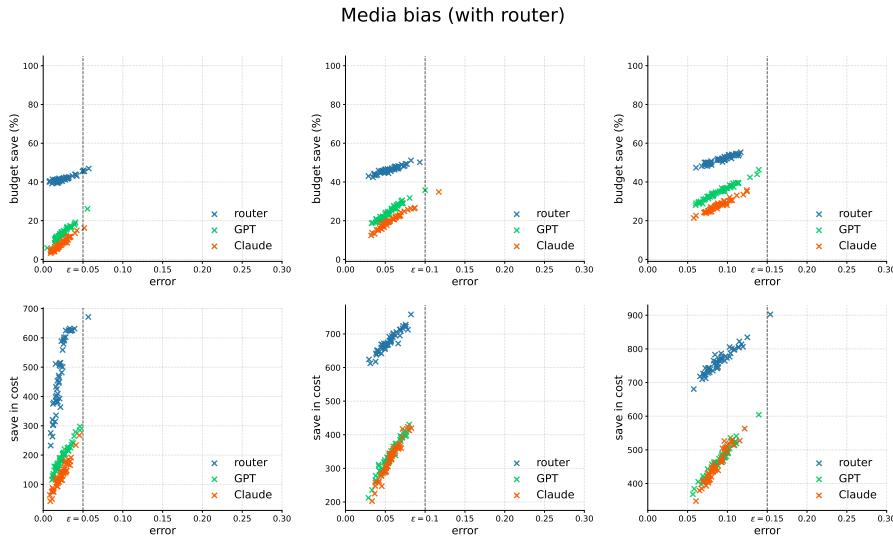
Incorporating costs. We also consider the cost-sensitive setting, where we take into account the costs of GPT-4o and Claude 3.7 Sonnet, and aim to minimize the overall labeling cost. We use the true current relative costs of the two models, setting $c_{\text{expert}} = 1$, $c_{\text{GPT}} = 0.25$, and $c_{\text{Claude}} = 0.075$. We show the results in Figure 3 (bottom) and Table 5 (bottom): cost-sensitive routing more than doubles the save in cost compared to GPT and more than triples the save compared to Claude.

5 DISCUSSION

This paper introduced probably approximately correct labels, a new approach to cost-sensitive dataset labeling assisted by off-the-shelf AI models and supported by rigorous statistical guarantees. Several directions for further development remain.

First, the procedure relies on a few user-specified hyperparameters—most notably the sample size m used to estimate the underlying loss and the choice of sampling weights. Although we outline sensible practical defaults, it would be valuable to develop optimal automatic methods for selecting these parameters.

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504 **Figure 3: PAC router for language models.** Realized error and save in budget for PAC labeling
505 with GPT, PAC labeling with Claude, and the PAC router between GPT and Claude. The top row
506 corresponds to the costless setting; the bottom row corresponds to the cost-sensitive setting. Each
507 column corresponds to a different value of ϵ (denoted by vertical dashed line).

510 Second, while the PAC labeling guarantee itself is agnostic to the quality of uncertainty scores,
511 our experiments show that good calibration is essential for achieving substantial budget saves. We
512 considered both simple, multicalibration-style approaches, as well as black-box approaches to un-
513 certainty calibration through the PAC router. One valuable direction for future work is to develop
514 provably optimal uncertainty calibration techniques.

515 Finally, an implicit assumption made throughout was that the expert labels are correct; all validity
516 claims are about agreement of the produced labels with expert labels. In practice, expert labels are
517 inevitably imperfect. Extending PAC labeling to account for noisy or heterogeneous expert sources
518 is an important direction for future work.

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756 A DEFERRED DETAILS
757758 A.1 PROOF OF THEOREM 1
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760 By the definition of u^* , we know $\frac{1}{n} \sum_{i=1}^n \ell(Y_i, \tilde{Y}_i) \leq \epsilon$ if $\tilde{Y}_i = Y_i \mathbf{1}\{U_i \geq u^*\} + \hat{Y}_i \mathbf{1}\{U_i < u^*\}$.
761 Furthermore, by monotonicity, for any labeling threshold $u' \leq u^*$ the error criterion is satisfied.
762 Therefore, on the event that $\hat{u} \leq u^*$, we know that $\frac{1}{n} \sum_{i=1}^n \ell(Y_i, \tilde{Y}_i) \leq \epsilon$.

763 We argue that $\mathbb{P}(\hat{u} \leq u^*) \geq 1 - \alpha$ as long as $\hat{L}^{U_i}(\alpha)$ are valid upper confidence bounds for all
764 U_i . Suppose not: suppose $\hat{u} > u^*$. By definition, this must mean that $\hat{L}^{u^*}(\alpha) \leq \epsilon$. But at the
765 same time, we know $L^{u^*} > \epsilon$; therefore, it must be that $\hat{L}^{u^*}(\alpha) < L^{u^*}$. This event happens with
766 probability at most α because $\hat{L}^{u^*}(\alpha)$ is a valid upper confidence bound, and thus we have shown
767 $\mathbb{P}(\hat{u} \leq u^*) \geq 1 - \alpha$.
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769 A.2 UNCERTAINTY MULTICALIBRATION
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771 Below we state the algorithm for calibrating uncertainty scores, building on the multicalibration
772 algorithm by Hébert-Johnson et al. (2018).
773

774 **Algorithm 2** Uncertainty multicalibration (Hébert-Johnson et al., 2018)

775 **Input:** uncertainties $U_1, \dots, U_m \in [0, 1]$, expert labels Y_1, \dots, Y_m , predicted labels $\hat{Y}_1, \dots, \hat{Y}_m$, clusters \mathcal{C} ,
776 number of bins B , tolerance $\tau > 0$
777 1: Define bins $b_j = [\frac{j-1}{B}, \frac{j}{B})$ for $j = 1, \dots, B$
778 2: **repeat**
779 3: updated \leftarrow **False**
780 4: **for** each cluster $C \in \mathcal{C}$ and each bin $j = 1, \dots, B$ **do**
781 5: Let $\mathcal{I}^{C,j} = \{i \in C : U_i \in b_j\}$
782 6: **if** $|\mathcal{I}^{C,j}| > 0$ **then**
783 7: Compute correction: $\Delta_{C,j} \leftarrow \frac{1}{|\mathcal{I}^{C,j}|} \sum_{i \in \mathcal{I}^{C,j}} (\mathbf{1}\{Y_i \neq \hat{Y}_i\} - U_i)$
784 8: **if** $|\Delta_{C,j}| > \tau$ **then**
785 9: Update: $U_i \leftarrow U_i + \Delta_{C,j}$ for all $i \in \mathcal{I}^{C,j}$
786 10: updated \leftarrow **True**
787 11: **until** updated is **False**
788 **Output:** calibrated uncertainties U_1, \dots, U_m

789 A.3 PAC ROUTER: DETAILS
790

791 Differentiating both sides of equation (4), we get
792

$$0 = \nabla_{\theta} \epsilon = \mathbb{E}_{X_i, Y_i} \left[\nabla_{\theta} \sum_{j=1}^k w_{\theta, j}(X_i) \cdot \ell(Y_i, \hat{Y}_i^j) \cdot \sigma(\tilde{u}(\theta) - U_i^j) \right]$$

$$= \mathbb{E}_{X_i, Y_i} \left[\sum_{j=1}^k \nabla_{\theta} w_{\theta, j}(X_i) \cdot \ell(Y_i, \hat{Y}_i^j) \cdot \sigma(\tilde{u}(\theta) - U_i^j) \right. \\ \left. + w_{\theta, j}(X_i) \cdot \ell(Y_i, \hat{Y}_i^j) \cdot \sigma(\tilde{u}(\theta) - U_i^j) \cdot (1 - \sigma(\tilde{u}(\theta) - U_i^j)) \cdot \nabla_{\theta} \tilde{u}(\theta) \right].$$

803 Rearranging, we get:

$$\nabla_{\theta} \tilde{u}(\theta) = - \frac{\mathbb{E}_{X_i, Y_i} \left[\sum_{j=1}^k \nabla_{\theta} w_{\theta, j}(X_i) \cdot \ell(Y_i, \hat{Y}_i^j) \cdot \sigma(u(\theta) - U_i^j) \right]}{\mathbb{E}_{X_i, Y_i} \left[\sum_{j=1}^k w_{\theta, j}(X_i) \cdot \ell(Y_i, \hat{Y}_i^j) \cdot \sigma(u(\theta) - U_i^j) \cdot (1 - \sigma(u(\theta) - U_i^j)) \right]}.$$

804 We can estimate the above gradient using a single expectation, by defining the probability distribution
805
806

$$807 \eta_{\theta}(X, Y, \hat{Y}, U, j) \propto p(X, Y) \cdot w_{\theta}(X)_j \cdot \ell(Y, \hat{Y}^j) \cdot \sigma(\tilde{u} - U^j) \cdot (1 - \sigma(\tilde{u} - U^j)),$$

810 where $p(X, Y)$ is the (fixed) empirical distribution of data points with corresponding labels, such
811 that

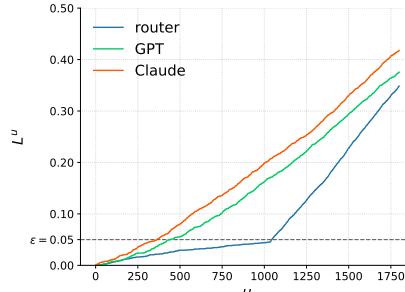
$$812 \quad 813 \quad \nabla_{\theta} \tilde{u}(\theta) = -\mathbb{E}_{X, Y, j \sim \eta_{\theta}(X, Y, \hat{Y}, U, j)} \left[\nabla_{\theta} \log w_{\theta}(X)_j \cdot \frac{1}{1 - \sigma(\tilde{u}(\theta) - U^j)} \right].$$

814 For the setting with learned uncertainties, following the same logic, we have implicit gradients:
815

$$816 \quad 817 \quad \nabla_{\theta} \tilde{u}(\theta, \gamma) = -\mathbb{E}_{X, Y, j \sim \eta_{\theta}} \left[\frac{\nabla_{\theta} \log w_{\theta, j}(X)}{1 - \sigma(\tilde{u}(\theta, \gamma) - U^j)} \right] \quad \text{and} \quad \nabla_{\gamma} \tilde{u}(\theta, \gamma) = \mathbb{E}_{X, Y, j \sim \eta_{\theta}} [\nabla_{\gamma} u_{\gamma, j}(X)].$$

819 A.4 LOSS L^u AFTER PAC ROUTING

820 We plot the loss $L^u = \frac{1}{n} \sum_{i=1}^n \ell^u(Y_i, \hat{Y}_i)$ that results from collecting labels at uncertainties greater
821 than or equal to u , as a function of u in the context of the PAC router application from Section 4. To
822 account for the fact that the different baselines might give uncertainties U_i of different magnitudes,
823 without loss of generality we first map the uncertainties to their respective rank in $\{1, \dots, n\}$. We
824 observe that the router produces a curve L^u that strictly dominates the loss curves of the individual
825 models. This means that, for any uncertainty threshold, the resulting labeling achieves a strictly
826 smaller error than with a single model. As a result, the critical uncertainty at which L^u crosses error
827 ϵ is significantly larger.
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839 Figure 4: **Loss L^u after PAC routing.** Error L^u after collecting labels at uncertainties greater than
840 or equal to u , as a function of u , for GPT and Claude individually and the PAC router. We observe
841 that the router achieves a lower error L^u than the individual baselines, for all u .
842

843 B DESCRIPTION OF PROTEIN FOLDING EXPERIMENT

844 Here, we briefly provide some background on the AlphaFold experiments performed in Section 4.
845 We first queried the UniProt (The UniProt Consortium, 2025) database for reviewed human proteins
846 for which 3D structures are available (`reviewed:true` and `structure_3d:true`). We then
847 used the SIFTS database to map UniProt IDs to specific Protein Data Bank (PDB) chains. Predicted
848 structures were retrieved from the AlphaFold Protein Structure Database (version 4) (Varadi et al.,
849 2022), while corresponding experimental structures were downloaded from PDB (Berman et al.,
850 2000). We then filtered and post-processed the chains and experimental structures using a basic
851 structural alignment pipeline.
852

853 Using this pipeline, we constructed a dataset of 6668 proteins. For each sourced protein, our dataset
854 contains (a) a sequence; (b) the experimental structure; (c) the predicted Local Distance Difference
855 Test (pLDDT), a measure of confidence that is generated by AlphaFold¹, and (d) the Root Mean
856 Square Deviation (RMSD), a measure of the ground-truth structural deviation between the predicted
857 and observed structures². Note that for proteins associated with multiple experimental structures,
858

859 ¹We refer the reader to <https://www.ebi.ac.uk/training/online/courses/alphafold/inputs-and-outputs/evaluating-alphafofolds-predicted-structures-using-confidence-scores/plddt-understanding-local-confidence/> for further background on pLDDT.

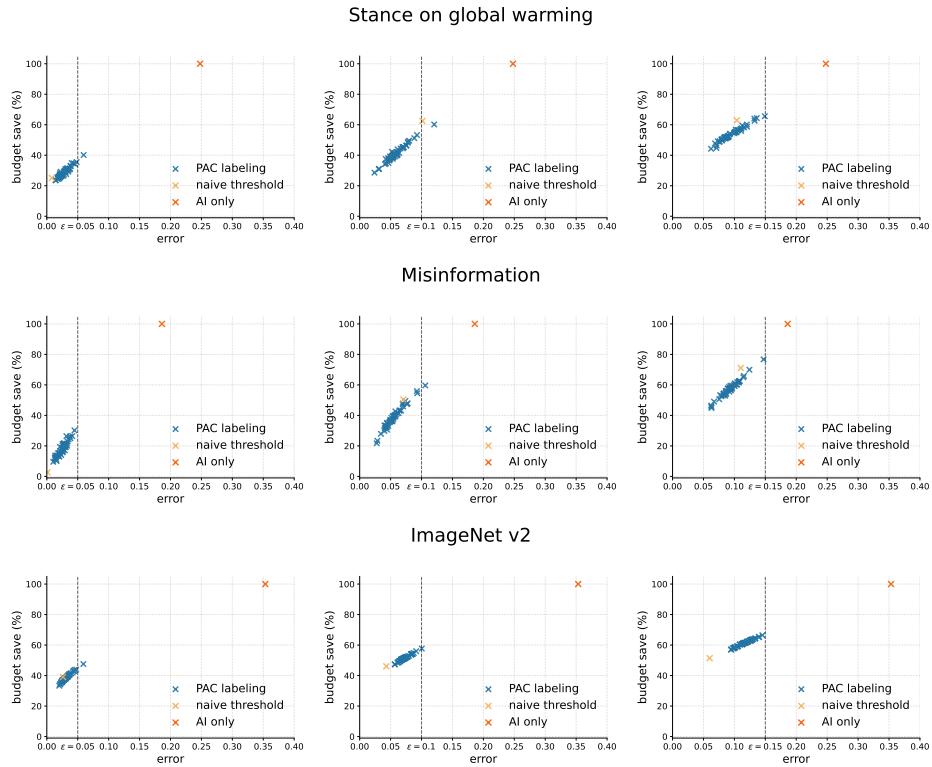
860 ²We refer the reader to <https://www.ebi.ac.uk/training/online/courses/alphafold/validation-and-impact/how-accurate-are-alphafofold-structure-predictions/> for further background on RMSD.

864 we computed the RMSD against all available chains and selected the instance yielding the minimum
 865 RMSD to represent the optimal experimental baseline.
 866

867 C ADDITIONAL EXPERIMENTAL RESULTS

868 C.1 DEFERRED PLOTS FROM THE MAIN TEXT

871 In Figure 5, we include plots analogous to those in Figure 1 for the remaining datasets: stance on
 872 global warming, misinformation, and ImageNet v2.
 873



890 **Figure 5: PAC labeling for discrete labels (additional datasets).** Realized error and save in budget
 891 for PAC labeling, the naive thresholding baseline, and the AI only baseline. Each row and column
 892 correspond to a different dataset and value of ϵ (denoted by vertical dashed line), respectively. For
 893 PAC labeling, we plot the realized error and save in budget for 50 randomly chosen trials. For the
 894 naive thresholding baseline, we collect expert labels for all points with $U_i \geq \epsilon$.
 895

900 C.2 EXPERIMENTS WITH ASYMPTOTIC CONFIDENCE INTERVALS

905 We include asymptotic analogues of the nonasymptotic results from Section 4. We rerun all experiments
 906 with discrete labels, this time using the asymptotic mean upper bound based on the central
 907 limit theorem (CLT) in the construction of PAC labels.
 908

911 In Table 6 and Table 7 we compare PAC labeling with asymptotic and nonasymptotic guarantees
 912 on text and image datasets, respectively. We see that asymptotic confidence intervals, in addition
 913 to being easier to implement, enable larger budget saves compared to nonasymptotic intervals. The
 914 downside of relying on asymptotic guarantees is that the error rates might be slightly inflated—
 915 throughout we see error rates slightly above the nominal 5%.

916 In Figure 6 we show the realized budget save against the realized error when we use asymptotic in-
 917 tervals. Overall we see similar trends as in Figure 1, however the weaker requirement of asymptotic
 918 validity allows for generally larger saves.
 919

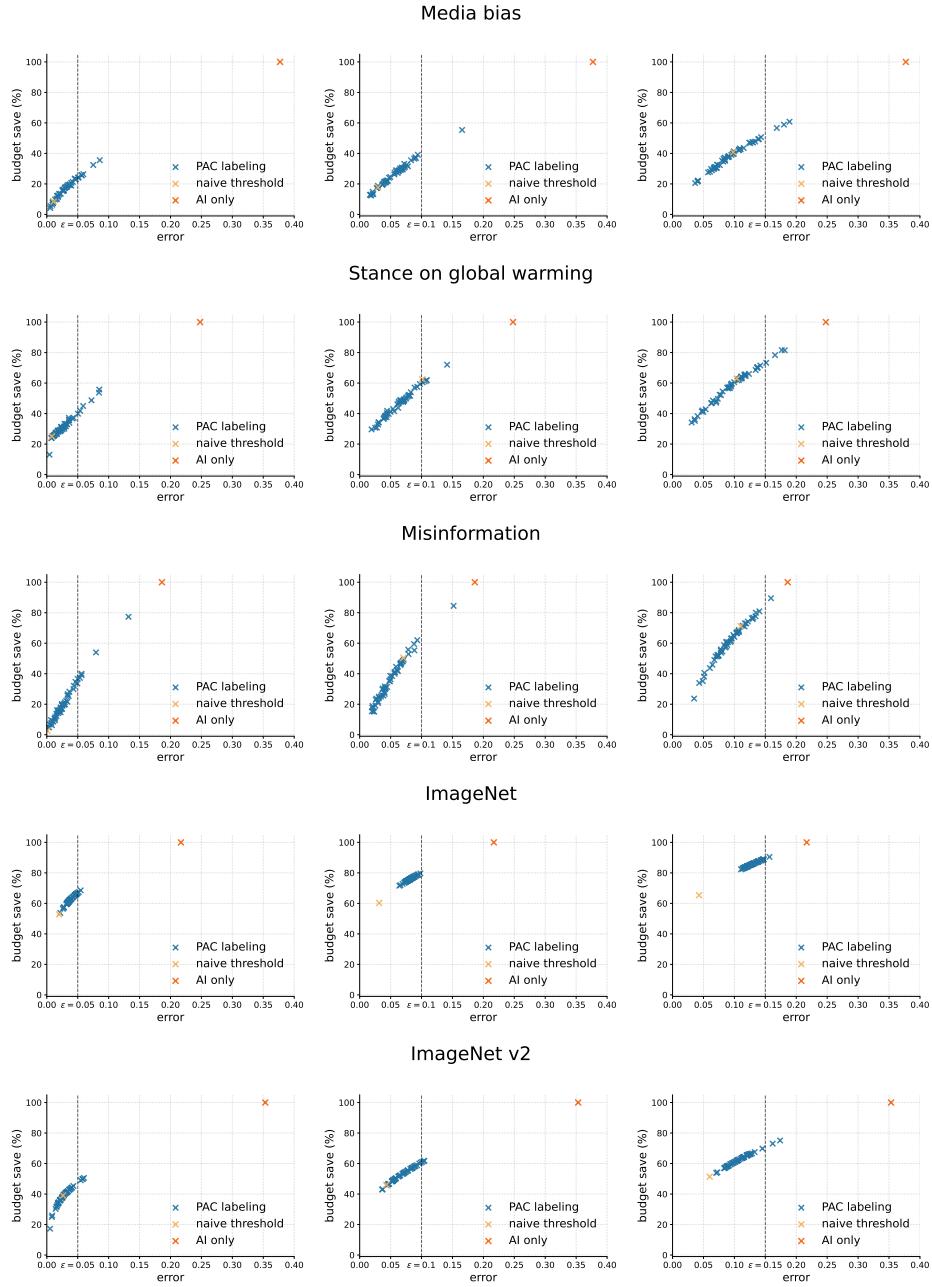


Figure 6: **PAC labeling for discrete labels with asymptotic confidence intervals.** Realized error and save in budget for PAC labeling, the naive thresholding baseline, and the AI only baseline. Each row and column correspond to a different dataset and value of ϵ (denoted by vertical dashed line), respectively. For PAC labeling, we plot the realized error and save in budget for 50 randomly chosen trials. For the naive thresholding baseline, we collect expert labels for all points with $U_i \geq \epsilon$.

C.3 EXPERIMENTS WITH VARYING m

Our PAC labeling algorithm (Algorithm 1) takes as input a sample size for estimation m . The choice of m should consider two criteria: first, m should be large enough such that estimating a one-dimensional mean with m samples is accurate, and second, m should be a relatively small fraction of the overall dataset size. The reason for the first criterion is that the procedure will be conservative, i.e. it will overcollect expert labels, if the upper confidence bound $\hat{L}^u(\alpha)$ is loose, which happens

972 973 974 975 976 977 978 979 980	Dataset	Metric	Method	
			PAC labeling (asymptotic)	PAC labeling (nonasymptotic)
981 982 983 984	Media bias	Budget save (%)	(16.11 \pm 6.96)%	(13.79 \pm 3.38)%
		Error	5.17%	4.10%
985 986 987 988 989 990 991	Stance on global warming	Budget save (%)	(32.15 \pm 7.38)%	(28.09 \pm 3.28)%
		Error	5.92%	4.57%
992 993 994 995 996 997 998 999 1000 1001 1002 1003 1004 1005 1006 1007 1008 1009 1010 1011 1012 1013 1014 1015 1016 1017 1018 1019 1020 1021 1022 1023 1024 1025	Misinformation	Budget save (%)	(21.41 \pm 10.95)%	(18.12 \pm 4.93)%
		Error	5.83%	3.80%

Table 6: **PAC labeling text datasets with GPT-4o, with asymptotic (left) and nonasymptotic (right) confidence intervals.** We set $\epsilon = 0.05$. PAC labeling with asymptotic guarantees enables larger saves, but may lead to slightly inflated error rates.

985 986 987 988 989 990 991	Dataset	Metric	Method	
			PAC labeling (asymptotic)	PAC labeling (nonasymptotic)
992 993 994 995 996 997 998 999 1000 1001 1002 1003 1004 1005 1006 1007 1008 1009 1010 1011 1012 1013 1014 1015 1016 1017 1018 1019 1020 1021 1022 1023 1024 1025	ImageNet	Budget save (%)	(62.82 \pm 2.57)%	(59.64 \pm 1.49)%
		Error	5.06%	4.73%
992 993 994 995 996 997 998 999 1000 1001 1002 1003 1004 1005 1006 1007 1008 1009 1010 1011 1012 1013 1014 1015 1016 1017 1018 1019 1020 1021 1022 1023 1024 1025	ImageNet v2	Budget save (%)	(39.20 \pm 5.82)%	(39.07 \pm 2.67)%
		Error	5.38%	4.74%

Table 7: **PAC labeling image datasets with ResNet-152, with asymptotic (left) and nonasymptotic (right) confidence intervals.** We set $\epsilon = 0.05$. PAC labeling with asymptotic guarantees enables larger saves, but may lead to slightly inflated error rates.

when m is small. At the same time, m being large means we are collecting many expert labels. Note that the two criteria do not depend on the specifics of the labeling problem much; to provide a heuristic that has robust performance for typical dataset sizes, we can take $m = \max\{500, 0.2n\}$.

In Figure 7, we plot the realized mean error and mean and standard deviation of the budget save for varying m and $\epsilon = 0.05$. We see that the budget save peaks around 500 for smaller datasets, while for ImageNet the save keeps increasing for larger m because $m = 2000$ is still negligible compared to the total dataset size.

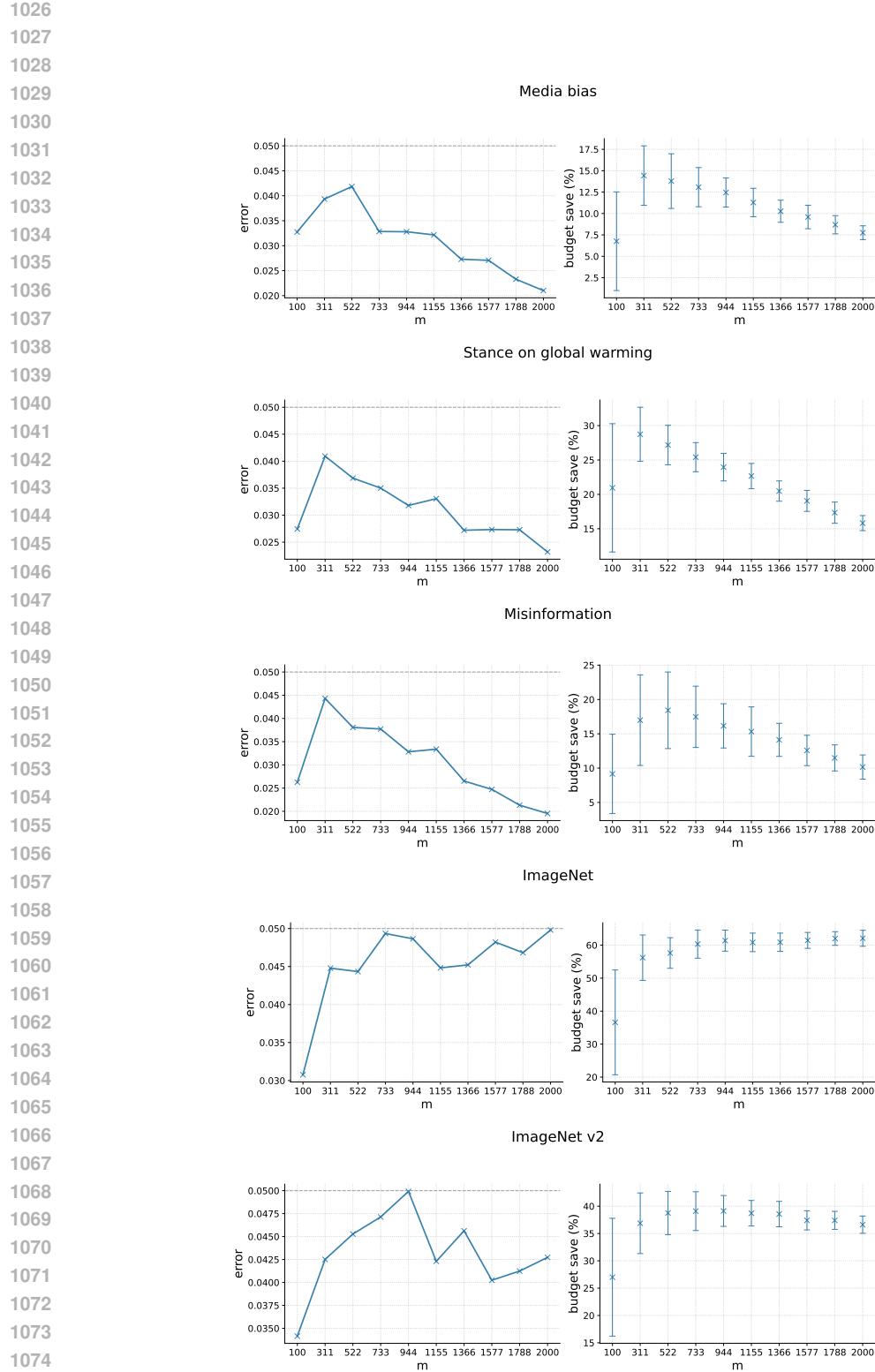


Figure 7: **Error and budget save for varying m .** Realized error and save in budget for PAC labeling with $\epsilon = 0.05$. Each row corresponds to a different dataset.