Active Assessment of Prediction Services as Accuracy Surface Over Attribute Combinations

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Abstract

Our goal is to evaluate the accuracy of a black-box classification model, not as 1 a single aggregate on a given test data distribution, but as a surface over a large 2 3 number of combinations of attributes characterizing multiple test data distributions. Such attributed accuracy measures become important as machine learning models 4 get deployed as a service, where the training data distribution is hidden from clients, 5 and different clients may be interested in diverse regions of the data distribution. 6 We present Attributed Accuracy Assay (AAA) - a Gaussian Process (GP)-based 7 probabilistic estimator for such an accuracy surface. Each attribute combination, 8 9 called an 'arm', is associated with a Beta density from which the service's accuracy 10 is sampled. We expect the GP to smooth the parameters of the Beta density over related arms to mitigate sparsity. We show that obvious application of GPs cannot 11 address the challenge of heteroscedastic uncertainty over a huge attribute space that 12 is sparsely and unevenly populated. In response, we present two enhancements: 13 pooling sparse observations, and regularizing the scale parameter of the Beta 14 densities. After introducing these innovations, we establish the effectiveness of 15 16 AAA both in terms of its estimation accuracy and exploration efficiency, through extensive experiments and analysis. 17

18 1 Introduction

Increasing concentration of big data and computing resources has resulted in widespread adoption of machine learning as a service (MLaaS). The best-performing NLP, speech, image and video recognition tools are now provided as network services. MLaaS comes with few accuracy specifications or service level agreements, perhaps only leaderboard numbers from benchmarks that may not be closely related to most clients' deployment data distributions. The client, therefore, finds it difficult to choose the best provider without extensive pilot trials [1]. Different clients may need to deploy the service on very different data distributions, with possibly widely different accuracy.

In such circumstances, we propose that a service provider, or a service standardization agency, publish 26 the accuracy of the classifier, not as one or few aggregate numbers, but as a surface defined on a space 27 of input instance attributes that capture the variability of consumer expectations. Indoor/outdoor, 28 day/night, urban/rural may be attributes of input images for visual object recognition tasks. Speaker 29 age, gender, ethnicity/accent may be attributes of input audio for speech recognition tasks. We call 30 31 a combination of attributes in their Cartesian space an *arm* (borrowing from bandit terminology) ¹. The labeled instances used by the service provider may not represent or cover well the space of 32 attributes of interest to subscribers. Labeled data may be proprietary and inaccessible to prospective 33 consumers and standardization agencies. Whoever estimates the accuracy surface, therefore, needs to 34 actively select instances from an unlabeled pool for labeling, presumably within a restricted budget, 35 to adequately cover the attribute space. 36

¹Figure 1 shows an example of diverse accuracy over arms.

³⁷ Several recent studies have highlighted the variability in accuracy across data sub-populations [2, 3],

specifically in the context of fairness [4, 5, 6], and also proposed active estimation techniques of

³⁹ sub-population accuracy [7, 8]. We solve a more general problem where the space of arms (sub-

40 population) defined by the Cartesian space of attributes grows combinatorially. This inevitably leads 41 to extreme sparsity of labeled instances for many arms. A central challenge is how to smooth the

estimate across related arms while faithfully representing the uncertainty for active exploration.

We present Attributed Accuracy Assay (AAA) — a practical system that estimates accuracy, together 43 with the uncertainty of the estimate, as a function of the attribute space. AAA uses these estimates 44 to drive the sampling policy for each attribute combination. Gaussian Process (GP) regression is a 45 natural choice to obtain smooth probabilistic accuracy estimates over arm attributes. However, a 46 straightforward GP model fails to address the challenge of heteroscedasticity that we face with uneven 47 and sparse supervision across arms. We model arm-specific service accuracy as drawn from a Beta 48 density that is characterized by mean and scale parameters, which are sampled from two GPs that are 49 informed by suitable trained kernels over the attribute space. We propose two further enhancements 50 to the training of this model. First, we recognize an over-smoothing problem with GP's estimation 51 of the Beta scale parameters, and propose a Dirichlet likelihood to supervise the relative values of 52 scale across arms. Second, we recognize that arms with very low support interfere with learning the 53 kernel parameters of the GPs. We mitigate this by pooling observations across related arms. With 54 these fixes, AAA achieves the best estimation performance among competitive alternatives. 55

Another practical challenge in our setting is that some attributes of instances are not known exactly. For example, attributes, such as camera shutter speed or speaker gender, may be explicitly provided as meta information attached with instances. But other attributes, such as indoor/outdoor, or speaker age, may have to be estimated noisily via another (attribute) classifier, because accurate human-based acquisition of attributes would be burdensome. AAA also tackles uncertain attribute inference. Its attribute classifiers are trained on a small amount of labeled data and their error rates are modeled in a probabilistic framework.

⁶³ We report on extensive experiments using several real data sets. Comparison with several estimators

- based on Bernoulli arm parameters, Beta densities per arm, and even simpler forms of GPs on the
- arm Beta distributions, shows that AAA is superior at quickly cutting down arm accuracy uncertainty.
- 66 Summarizing, our contributions are:
- We motivate and define the problem of accuracy surface estimation over a large space of attribute combinations.
- Our proposed estimator AAA fits a Beta density for every attribute combination (arm), with its
 parameters smoothed via two GPs to capture heteroscedastic uncertainty of each arm's accuracy
 under limited data settings.
- We propose two important components included in AAA: 1) a Dirichlet regularization to control over-smoothing of the Beta scale parameters, and 2) pooled observations to reduce over-fitting of a GP-associated kernel to sparse arms.

 We show significant gains in terms of both estimation quality and the efficiency of exploration on four real classification models compared to existing methods. AAA obtains an average 80%

reduction in macro averaged square error over the existing methods.

78 2 Problem Setup

⁷⁹ Our goal is to evaluate a given machine learning service model S used by a diverse set of consumers. ⁸⁰ The service $S : \mathcal{X} \mapsto \mathcal{Y}$ could be any predictive model that, for an input instance $\mathbf{x} \in \mathcal{X}$, assigns ⁸¹ an output label $\hat{y} \in \mathcal{Y}$, where \mathcal{Y} is a discrete label space. Let $y(\mathbf{x})$ denote the true label of \mathbf{x} and ⁸² Agree (y, \hat{y}) denote the match between the two labels. For scalar classification, Agree (y, \hat{y}) is in ⁸³ {0,1}. For structured outputs, e.g., sequences, we could use measures like BLEU scores in [0,1]. ⁸⁴ Classifiers are routinely evaluated on their expected accuracy on a data distribution $P(\mathcal{X}, \mathcal{Y})$:

$$\rho = \mathbb{E}_{P(\mathbf{x}, y)}[\text{Agree}(y, S(\mathbf{x}))] \tag{1}$$

We propose to go beyond this single measure and define accuracy as a surface over a space of attributes of the input instances. Let A denote a list of K attributes that capture the variability of consumer expectation on which the service S will be deployed. For instance, visual object recognition is affected by the background scene, and facial recognition is affected by demographic attributes. We use $A(\mathbf{x}) \in \mathcal{A}$ to denote the vector of values of attributes of input \mathbf{x} and \mathcal{A} to denote the Cartesian

- ⁹⁰ product of the domains of all attributes. An attribute could be discrete, e.g., the ethnicity of a speaker;
- Boolean, e.g., whether a scene is outdoors/indoors; or continuous, e.g., the age of the speaker in
- speech recognition. Some of the attributes of \mathbf{x} , for example the camera settings of an image, may be known exactly, and others may only be available as a distribution $M_k(a_k|\mathbf{x})$ for an attribute $a_k \in A$,

obtained from a pre-trained probabilistic classifier.

- Generalizing from a single global expected accuracy (1), we define the accuracy surface $\rho : \mathcal{A} \to [0, 1]$
- 96 of a service S at each attribute combination $a \in A$, given a data distribution $P(\mathcal{X}, \mathcal{Y})$, as

$$\rho(\boldsymbol{a}) = \mathbb{E}_{P(\mathbf{x}, y|A(\mathbf{x})=\boldsymbol{a})}[\text{Agree}(y, S(\mathbf{x}))]$$
(2)

97 Our goal is to provide an estimate of $\rho(a)$ given two kind of data sampled from $P(\mathcal{X}, \mathcal{Y})$: a small

 $_{98}$ labeled sample D, and a large unlabeled sample U. In addition, we are given a budget of B instances

for which we can seek labels y from a human by selecting them from U. Applying M_k to all of U is, however, free of cost.

We aim to design a probabilistic estimator for $\rho(a)$, which we denote as $P(\rho|a)$ where $\rho \in [0, 1]$ and $a \in A$. This is distinct from active learning, which selects instances to train the learner toward greater accuracy, and also active accuracy estimation [7], which does not involve a surface over as. We also show that standard tools to regress from a to ρ are worse than our proposal.

We measure the quality of our estimate as the square error between the gold accuracy $\rho(a)$ and the mean of the estimated accuracy distribution $P(\rho|a)$. Our estimator distribution naturally gives an idea of the posterior variance of accuracy estimate of each attribute combination, which we use for uncertainty-based exploration.

109 3 Proposed Estimator

We will first review recent work that leads to candidate solutions to our problem, discuss their limitations, and finally present our solution. Initially, to keep the treatment simple, we assume $A(\mathbf{x})$ and gold y (hence c = Agree(S(x), y), the service correctness bit) is known for all instances. Later in this section, we remove these assumptions.

The simplest option is to ignore any relationship between arms, and, for each arm a, fit a suitable density over $\rho(a)$. When this density is sampled, we get a number in [0, 1], which is like a coin head probability used to sample correctness bits c. For representing uncertainty of accuracy values (which are ratios between two counts), the Beta distribution $\mathfrak{B}(\cdot, \cdot)$ is a natural choice. We call this baseline method **Beta-I**.

The variance of the estimated Beta density can be used for actively sampling arms. Ji et al. [7] describe a related scenario, stressing on active sampling. However, this approach cannot share observations or smooth the estimated density at a sparsely-populated arm with information from similar arms. In our real-life scenario, we expect accuracy surface smoother and the number of arms to be large enough that many arms will get very few, if any, instances.

The second baseline method, which we call **BernGP**, is to view the (a, c) instances in D as a standard classification data set with the binary c values as class label and a as input features. Given the limited data, we can use the well-known GP classification approach [9] for fitting smooth values ρ as a function of a. Suppose the arms a can be embedded to $\mathcal{V}(a)$ in a suitable space induced by some similarity kernel. In this embedding space, we expect the accuracy of S to vary smoothly. Given a kernel $K_1(a, a')$ to guide the extent of sharing of information across arms, a standard form of this GP would be

$$P(c|\boldsymbol{a}) = \text{Bernoulli}(c; \text{sigmoid}(f_{\boldsymbol{a}})); \quad f \sim GP(0, K_1).$$
(3)

The GP can give estimates of uncertainty of $\rho(a)$, which may be used for active sampling of arms.

As we will demonstrate, such GP-imposed estimate of uncertainty of $\rho(a)$ is inadequate, because it loses sight of the number of supporting observations at each arm, which could be very diverse. This is because the standard GP assumption of homoscedasticity, that is, identical noise around each arm is violated when observations per arm differ significantly. We therefore need a mechanism to separately account for the uncertainty at each arm, even the unexplored ones, to guide the strategy for actively collecting more labeled data.

138 3.1 The basic BetaGP proposal

We model arm-specific noise by allowing each arm to represent the uncertainty of ρ_a , not just by an underlying GP as in BernGP above, but also by a separate scale parameter. Further, the scale parameter is smoothed over neighboring arms using another GP. The influence of this scale on the

uncertainty of ρ_a is expressed by a Beta distribution as follows:

$$P(\rho|\boldsymbol{a}) \sim \mathfrak{B}(\rho; \phi(f_{\boldsymbol{a}}), \psi(g_{\boldsymbol{a}})) \tag{4}$$

$$\phi(f_a) = \text{sigmoid}(f_a), \qquad f \sim GP(0, K_1), \tag{5}$$

$$\psi(g_a) = \log(1 + e^{g_a}), \qquad g \sim GP(0, K_2),$$
(6)

where we use $\phi(\bullet), \psi(\bullet)$ to denote the parameters of the Beta distribution at arm a. The Beta distribution is commonly represented via α, β parameters whereas we chose the less popular mean (ϕ) and scale (ψ) parameters. While these two forms are functionally equivalent with $\phi = \frac{\alpha}{\alpha + \beta}, \psi = \frac{1}{\alpha}$

¹⁴⁶ $\alpha + \beta$, we preferred the second form because imposing GP smoothness across arms on the mean ¹⁴⁷ accuracy and scale seemed more meaningful. We validate this empirically in the Appendix.

Two kernel functions $K_1(a, a')$, $K_2(a, a')$ defined over pairs of arms $a, a' \in \mathcal{A}$ control the degree of smoothness among the Beta parameters across the arms. We use an RBF kernel defined over learned shared embeddings $\mathcal{V}(a)$:

$$K_1(\boldsymbol{a}, \boldsymbol{a}') = s_1 \exp\left[-\frac{\|\mathcal{V}(\boldsymbol{a}) - \mathcal{V}(\boldsymbol{a}')\|^2}{l_1}\right], \qquad K_2(\boldsymbol{a}, \boldsymbol{a}') = s_2 \exp\left[-\frac{\|\mathcal{V}(\boldsymbol{a}) - \mathcal{V}(\boldsymbol{a}')\|^2}{l_2}\right]$$
(7)

where s_1, s_2, l_1, l_2 denote the scale and length parameters of the two kernels. The scale and length parameters are learned along with the parameters of embeddings $\mathcal{V}(a)$ during training.

Initially, we assume we are given a labeled dataset $D = \{(\mathbf{x}_i, \mathbf{a}_i, y_i) : i = 1..., I\}$ with attribute information available. Using predictions from the classification service S, we associate a 0/1 accuracy $c_i = \text{Agree}(y_i, S(\mathbf{x}_i))$. We can thus extend D to $\{(\mathbf{x}_i, \mathbf{a}_i, y_i, c_i) : i \in [I]\}$.

Let $c_a = \sum_{i:A(\mathbf{x}_i)=a} c_i$ denote the total accuracy score in arm a. Let n_a denote the total number of labeled examples in arm a. The likelihood of all observations given functions f, g decomposes as a product of Beta-binomial² distributions at each arm as follows:

$$\Pr(D|f,g) = \prod_{\boldsymbol{a}} \int_{\rho} \rho^{c_{\boldsymbol{a}}} (1-\rho)^{n_{\boldsymbol{a}}-c_{\boldsymbol{a}}} \mathfrak{B}(\rho|\phi(f_{\boldsymbol{a}}),\psi(g_{\boldsymbol{a}}))) \mathrm{d}\rho.$$
(8)

$$=\prod_{a} \frac{\mathcal{B}(\phi(f_{a})\psi(g_{a}) + c_{a}, (1 - \phi(f_{a}))\psi(g_{a}) + n_{a} - c_{a})}{\mathcal{B}(\phi(f_{a})\psi(g_{a}), (1 - \phi(f_{a}))\psi(g_{a}))},$$
(9)

where B is the Beta function, and the second expression is a rewrite of the Beta-binomial likelihood.

During training we calculate the posterior distribution of functions f, g using the above data likelihood 160 $\Pr(D|f,g)$ and GP priors given in eqns. (5) and (6). The posterior cannot be computed analytically 161 given our likelihood, so we use variational methods. Further, we reduce the $\mathcal{O}(|\mathcal{A}|^3)$ complexity of 162 posterior computation, using the inducing point method of Hensman et al. [9], whereby we learn 163 m locations $\mathbf{u} \in \mathbb{R}^{d \times m}$, mean $\mu \in \mathbb{R}^m$, and covariance $\Sigma \in \mathbb{R}^{m \times m}$ of inducing points. Doing 164 so brings down the complexity to $\mathcal{O}(m^2|\mathcal{A}|), m \ll |\mathcal{A}|$. These parameters are learned end to end 165 with the parameters of the neural network used to extract embeddings $\mathcal{V}(a)$ of arms a, and kernel 166 parameters s_1, s_2, ℓ_1, ℓ_2 . We used off-the-shelf Gaussian process library: GPyTorch [10] to train the 167 above likelihood with variational methods. Details of this procedure can be found in the Appendix. 168 We denote the posterior functions as P(f|D), P(g|D). Thereafter, the mean estimated accuracy for 169 an arm *a* is computed as 170

$$\mathbb{E}(\rho|\boldsymbol{a}) = \mathbb{E}_{f \sim P(f|D)}[\phi(f_{\boldsymbol{a}})].$$
(10)

We call this setup **BetaGP**. Next, we will argue why BetaGP still has serious limitations, and offer mitigation measures.

173 **3.2** Supervision for scale parameters

We had introduced the second GP g_a to model arm-specific noise, and similar techniques have been

proposed earlier by Lázaro-Gredilla and Titsias [11], Kersting et al. [12], Goldberg et al. [13], but for heteroscedasticity in Gaussian observations. However, we found the posterior distribution of

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²The $\binom{n_a}{c_a}$ term does not apply since we are given not just counts but accuracy c_i of individual points.

scale values $\psi(g_a)$ at each arm tended to converge to similar values, even across arms with orders of magnitude difference in number of observations n_a . On hindsight, that was to be expected, because the data likelihood (8) increases monotonically with scale ψ_a . The only control over its converging to ∞ is the GP prior $g \sim GP(0, K_2)$. In the Appendix, we illustrate this phenomenon with an example. We propose a simple fix to the scale supervision problem. We expect the relative values of scale across arms to reflect the distribution of the proportion of observations $\frac{n_a}{n}$ across arms (with $n = \sum_a n_a$). We impose a joint Dirichlet distribution using the scale of arms $\psi(g_a)$ as parameters, and write the likelihood of the observed proportions as (with Γ denoting Gamma function):

$$\log \Pr(\{n_{\boldsymbol{a}}\}|g) = \sum_{\boldsymbol{a}} ((\psi(g_{\boldsymbol{a}}) - 1)\log \frac{n_{\boldsymbol{a}}}{n} - \log \Gamma(\psi(g_{\boldsymbol{a}})) + \log \Gamma(\sum_{\boldsymbol{a}} \psi(g_{\boldsymbol{a}}))$$
(11)

We call this **BetaGP-SL**. With this as an additional term in the data likelihood, we obtained significantly improved uncertainty estimates at each arm, as we will show in the experiment section.

187 3.3 Pooling for sparse observations

Recall that the observations are accumulation of 1/0 agreement scores for all instances that belong to 188 an arm. Given the nature of our problem, arms have varying levels of supervision, and also highly 189 varying true accuracy values. Even when the available labeled data is large, many arms will continue 190 to have sparse supervision because they represent rare attribute combinations. The combination 191 of high variance observations and sparse supervision could lead to learning of non-smooth kernel 192 parameters. The situation is further aggravated when learning a deep kernel. This problem has 193 resemblance to "collapsing variance problem" [14] such as when Gaussian Mixture models overfit on 194 outliers or when topic models overfit a noisy document in the corpus. Instead of depending purely 195 on GP priors to smooth over these noisy observations, we found it helpful to also externally smooth 196 noisy observations. For each arm a with observations below a threshold, we mean-pool observations 197 from some number of nearest neighbors, weighted by their kernel similarity with a. We will see that 198 such external smoothing resulted in significantly more accurate estimates particularly for arms with 199 extreme accuracy values. We call this method BetaGP-SLP (note that this also includes the scale 200 supervision objective described in the previous section). Two other mechanisms take us to the full 201 form of the AAA system, which we describe next. 202

203 3.4 Exploration

The variance estimate of an arm informs its uncertainty and is commonly used for efficient exploration [15]. Let P(f|D), P(g|D) denote the learned posterior distribution of the GPs. Using these, the estimated variance at an arm is given as:

$$\mathbb{V}(\rho|\boldsymbol{a}) = \mathbb{E}_{f \sim P(f|D), g \sim P(g|D)} \left[\int_{\rho} (\rho - \mathbb{E}(\rho|\boldsymbol{a}))^2 \mathfrak{B}(\rho; \phi(f_{\boldsymbol{a}}), \psi(g_{\boldsymbol{a}})) \mathrm{d}\rho \right]$$
(12)

where the expected value is given in eqn. (10). We use sampling to estimate the above expectation. The arm to be sampled next is chosen as the one with the highest variance among unexplored arms. We then sample an unexplored example with highest affiliation ($P(\mathbf{a} \mid \mathbf{x})$) with the chosen arm.

210 3.5 Modeling Attribute Uncertainty

Recall that attributes of an instance \mathbf{x} are obtained from models $M_k(a_k|\mathbf{x})$, $k \in [K]$, which may be highly noisy for some attributes. Thus, we cannot assume a fixed attribute vector $A(\mathbf{x})$ for an instance \mathbf{x} . We address this by designing a model that can combine these noisy estimates into a joint distribution $P(\mathbf{a}|\mathbf{x})$ using which, we can fractionally assign each instance \mathbf{x}_i across arms. A baseline model for $P(\mathbf{a}|\mathbf{x})$ would be just the product $\prod_{k=1}^{K} M_k(a_k|\mathbf{x})$. However, we expect values of attributes to be correlated (e.g. attribute 'high-pitch' is likely to be correlated with gender 'female'). Also, the probabilities $M_k(a_k|\mathbf{x})$ may not be well-calibrated.

We therefore propose an alternative joint model that can both recalibrate individual classifiers via temperature scaling [16], and model their correlation. We have a small seed labeled dataset D with gold attribute labels, independent noisy distributions from each attribute model $M_k(a_k|\mathbf{x})$, and an unlabeled dataset U. We prefer simple factorized models. We factorize log $Pr(\mathbf{a}|\mathbf{x})$ as a sum of temperature-weighted logits and a joint (log) potential as shown in expression (13) below.

$$\log \Pr(\mathbf{a}|\mathbf{x}) = \log \Pr(a_1, a_2, \cdots, a_K | \mathbf{x}) = \sum_{k=1}^{K} t_k \log M_k(a_k | \mathbf{x}) + N(a_1, a_2, \cdots, a_K)$$
(13)

Here N denotes a dense network to model the correlation between attributes, and t_1, \ldots, t_K denote the temperature parameters used to rescale noisy attribute probabilities. The maximum likelihood over D is $\max_{t,N} \sum_{(\mathbf{x}_i, \mathbf{a}_i) \in D} \log \Pr(\mathbf{a}_i | \mathbf{x}_i)$

$$= \max_{t,N} \sum_{\mathbf{x}_i \in D} \left\{ \sum_{k=1}^{K} t_k \log M_k(a_{ik} | \mathbf{x}_i) + N(a_{i1}, \dots a_{iK}) - \log(Z_i) \right\}$$
(14)

²²⁶ Z_i denotes the partition function for an example \mathbf{x}_i which requires summation over \mathcal{A} . It could ²²⁷ be intractable to compute Z_i exactly when \mathcal{A} is large. In such cases, Z_i can be approximated by ²²⁸ sampling. In our case, we could get exact estimates.

In addition to D, we use the unlabeled instances U with predictions from attribute predictors filling the role of gold-attributes. Details on how we train the parameters on large but noisy U and small but correct D can be found in the Appendix.

The estimation method of BetaGP-SLP with variance based exploration and calibration described here constitute our proposed estimator: AAA. Detailed pseudo-code of AAA is given in the Appendix.

234 4 Experiments

Our exploration of various methods and data sets is guided by the following research questions.

- How do various methods for arm accuracy estimation compare?
- To what extent do BetaGP, scale supervision and pooled observations help beyond BernGP?
- For the best techniques from above, how do various active exploration strategies compare?
- How well does our proposed model of attribute uncertainty work?

240 4.1 Data sets and tasks

We experiment with two real data sets and tasks. Our two tasks are male-female gender classification with two classes and animal classification with 10 classes.

Male-Female classification (MF): CelebA [17] is a popular celebrity faces and attribute data set 243 which identifies the gender of celebrities among 39 other binary attributes. The label is gender. The 244 accuracy surface spans various demographic, style, and personality related attributes. We hand-pick 245 a subset of 12 attributes that we deem important for gender classification. Gender-neural attributes 246 such as wearing spectacles or hat are ignored (see Appendix for more details). A subset of 50,000 247 248 examples is used to train classifiers on each of the 12 attributes using a pretrained ResNet-50 model. The remaining 150,000 examples in the data set are set as the unlabeled pool from which we actively 249 explore new examples for human feedback. 250

Animal classification (AC): COCO-Stuff [18] provides an image collection. For each image, labels for foreground (cow, camel) and background (sky, snow, water) 'stuff' are available. Visual recognition models often correlate the background scene with the animal label such as camel with deserts and cow with meadows. Thus, foreground stuff labels are our regular *y*-labels while background stuff labels supply our notion of attributes.

We collapse fine stuff labels into five coarse labels using the dataset provided label hierarchy. These are: water, ground, sky, structure, furniture. The Coco dataset has around 90 object labels. Here we use a subset of 10 labels corresponding to animals. We take special care to filter out images with multiple/no animals and adapt the pixel segmentation/classification task to object classification (see the Appendix for more details). The image is further annotated with the five binary labels corresponding to five coarse stuff labels. The scene descriptive five binary labels and ten object labels make up for $32 \times 10 = 320$ attribute combinations.

263 4.2 Service Models

For the MF task, we use two service models S. **MF-CelebA** is a service model for gender classification. To simulate separate D and U, it is trained on a random subset of CelebA with a ResNet-50



$Service \rightarrow$	AC-COCOS10K	AC-COCOS	MF-IMDB	MF-CelebA
CPredictor	5.4 / 15.0	3.2/9.4	1.2 / 8.2	5.2 / 35.9
Beta-I	7.0 / 15.6	4.3 / 10.0	1.6 / 8.4	4.7 / 30.3
BernGP	7.0 / 13.2	3.5 / 8.6	1.7 / 7.6	4.9 / 28.1
BetaGP	7.1 / 14.3	3.3 / 7.9	2.2 / 6.6	4.6 / 25.9
BetaGP-SL	5.3 / 11.7	2.8/6.8	1.4 / 4.4	4.1 / 22.6
BetaGP-SLP	4.7 / 10.4	2.8 / 5.7	1.4 / 3.9	4.3 / 23.3

Figure 1: Macro and micro averaged accuracy (right most) and ten quantiles (x-axis) of per-arm accuracy (y-axis).

Table 2: Comparing different estimation methods on labeled data size 2000 across four tasks. No exploration is involved. Each cell shows two numbers in the format "macro MSE / worst MSE" obtained over three runs. BetaGP-SLP generally gives the lowest MSE.

model. MF-IMDB is a publicly available³ classifier trained on IMBD-Wiki dataset, also using the
 ResNet50 architecture. The attribute predictors are trained using ResNet-50 on a subset of the CelebA
 dataset for both service models.

For the AC task, we use two publicly available⁴ service models S. AC-COCOS was trained on 269 COCOS data set with 164K examples. AC-COCOS10k was trained on COCOS10K, an earlier 270 version of COCOS with only 10K instances. We use these architectures for both label and attribute 271 prediction. See Appendix for more details on attribute predictor, service models and their architecture. 272 273 In Figure 1, we illustrate some statistics of the shape of the accuracy surface for the four dataset-task combinations. Although S's mean accuracy (right most bars) is reasonably high, the accuracy of the 274 arms in the 10% quantile is abysmally low, while arms in the top quantiles have near perfect accuracy. 275 This further motivates the need for an accuracy surface instead of single accuracy estimate. 276

277 4.3 Methods Compared

We compare the proposed estimation method AAA against natural baselines, alternatives, and 278 ablations. Some of the methods, such as Beta-I, BernGP and BetaGP, we have already defined in 279 Section 3. We train methods BernGP and BetaGP using the default arm-level likelihood. We also 280 separately evaluate the impact of our fixes on BetaGP with only scale supervision: BetaGP-SL and 281 along with mean pooling: **BetaGP-SLP**. We also include a trivial baseline: **CPredictor** which fits 282 all the arms with a global accuracy estimated using gold D. We do not try sparse observation pooling 283 with Beta-I since there is no notion of per-arm closeness. We also skip it on BernGP since it is worse 284 than BetaGP as we will show below. 285

286 4.4 Other experimental settings

Gold accuracies $\rho(a)$: We compute the oracular accuracy per arm using the gold attribute/label values of examples in U which we treat as unlabeled during exploration. For every arm with at least five examples, we set its accuracy to be the empirical estimate obtained through the average correctness of all the examples that belong to the arm. We discard and not evaluate on any arms with fewer than five examples since their true accuracy cannot reliably be estimated.

Warm start: We start with 500 examples having gold attributes+labels to warm start all our experiments. The random seed also picks this random subset of 500 labeled examples. We calculate the overall accuracy of the classifier on these warm start examples as $\hat{\rho} = (\sum_i c_i)/(\sum_i 1)$. For all arms we use a default smoothing to $[\lambda \hat{\rho}, \lambda]$ where $\lambda = 0.1$, a randomly picked low value.

Unless otherwise specified, we give equal importance to each arm and report MSE macroaveraged over all arms. Along with macro MSE, we also sometimes report MSE on the subset of 50 worst accuracy arms, referred to as worst MSE. We report other aggregate errors in the Appendix. All the numbers reported here are averaged over three runs with different random seeds. The initial set of warm-start examples (D) is also changed between the runs. In the case of BetaGP-SLP, for any arm with observation count below 5, we mean pool from its three closest neighbours.

In the following Sections: 4.5 and 4.6, we compare various estimation and exploration strategies with $P(\mathbf{a}|\mathbf{x})$ noise calibrated as described in Section 3.5. In Section 4.7, we study different forms of calibration and demonstrate the superiority of our proposed calibration technique of Equation (13).

³https://github.com/yu4u/age-gender-estimation

⁴https://github.com/kazuto1011/deeplab-pytorch/



Figure 3: Comparison of estimation methods using worst MSE metric. The shaded region shows standard error. BetaGP-SLP consistently performs better than BetaGP. Beta-I is worse than its smoother counterparts.



Figure 4: Comparison of exploration methods. BetaGP-SLP reduces macro MSE fastest most of the time. Shaded region shows standard error.



Figure 5: Calibration methods compared on different tasks. Cal:Full (red) includes temperature-based recalibration and correlation modeling with joint potential and gives the best macro MSE. Shaded region shows standard error.

305 4.5 Accuracy Estimation Quality

We evaluate methods on their estimation quality when each method is provided with exactly the 306 same (randomly chosen) labeled set. We compare the four service models when fitted on labeled 307 data of size 2,000 and the results appear in Table 2. Note that we only have label supervision on \mathcal{Y} 308 in the labeled data. Table 2 shows macro and worst MSE, standard deviation for each metric can 309 be found in Appendix. In Figure 3, we show worst MSE for a range of labeled data sizes along 310 with their error bars. We make the following observations. **Smoothing helps:** Since we have a large 311 number of arms, we expect Beta-I to fare worse than its smooth counterparts (BernGP and BetaGP), 312 especially on the worst arms. This is confirmed in the table. In three out of four cases, this method 313 is worse than even the constant predictor CPredictor on both metrics. Modeling arm specific noise 314 helps: BetaGP is better than BernGP on almost all the cases in the table. Significant gains when 315 the scale supervision problem of BetaGP is fixed: BetaGP-SL is significantly better than BetaGP 316 317 in the table and figure. **Our pooling strategy helps:** BetaGP-SLP improves BetaGP-SL over worst MSE without hurting macro MSE as seen in the table and figure. 318

319 4.6 Exploration Efficiency

We compare different methods that use their own estimated variance for exploring instances to 320 label (Section 3.4), as a function of the number of explored examples — see Figure 4. In most 321 cases, BetaGP-SLP gives the smallest macro MSE, beating Beta-I and BetaGP. Note Beta-I is the 322 exploration method recently suggested in [7]. We observe that BetaGP provides very poor exploration 323 quality, indicating that the uncertainty of arms is not captured well by just using two GPs. In fact, 324 in many cases BetaGP is worse than Beta-I, even though we saw the opposite trend in estimation 325 quality (Figure 3). These experiments brings out the significant role of Dirichlet scale supervision 326 and pooled observations in enhancing the uncertainty estimates at each arm. 327

328 4.7 Impact of Calibration

We consider two baselines along with our method explained in Section 3.5: **Cal:Raw**, which uses the predicted attribute from the attribute models without any calibration and **Cal:Temp**, which calibrates only the temperature parameters shown in eqn. (13), i.e., without the joint potential part. We refer to our method of calibration using temperature and joint potentials as **Cal:Full**. We compare these on the four tasks with estimation method set to Beta-I and random exploration strategy. Figure 5 compares the three methods: Cal:Raw(Black), Cal:Temp(Blue), Cal:Full(Red). The X-axis is the number of explored examples beyond *D*, and Y-axis is estimation error. Observe how Cal:Temp and Cal:Full are consistently better than Cal:Raw, and Cal:Full is better than Cal:Temp.

337 5 Related Work

Our problem of actively estimating the accuracy *surface* of a classifier generalizes the more estab-338 lished problem of estimating a single accuracy score [19, 20, 21, 22, 23, 24]. For that problem, a 339 known solution is stratified sampling, which partitions data into homogeneous strata and then seeks 340 examples from regions with highest uncertainty and support. If we view each arm as a stratum, our 341 method follows similar strategy. A key difference in our setting is that low support arms cannot be 342 ignored. This makes it imperative to calibrate well the uncertainty under limited and skewed support 343 distribution. The setting of Ji et al. [7] is the closest to ours. However, their work only considers a 344 single attribute which they fit using Beta-I, whereas we focus on the challenges of estimating accuracy 345 over many sparsely populated attribute combinations. 346

Sub-population performance: Several recent papers have focused on identifying sub-populations 347 with significantly worse accuracy than aggregated accuracy [2, 3, 6, 8, 25, 26]. Some of these have 348 349 also proposed sample-efficient techniques [6, 8] for estimation of performance on specific sub-groups, such as the ones defined by attributes like gender and race. Our accuracy surface estimation problem 350 can be seen as a generalization where we need to estimate for all sub-groups defined in the Cartesian 351 space of pre-specified semantic attributes. Mitchell et al. [5] recommend enclosing model cards with 352 released or deployed models. In model cards, they suggest reporting performance under various 353 relevant demographic/environmental factors which resembles the accuracy surface. 354

Experiment design: Another related area is experiment design using active explorations with GPs 355 [27]. Their goal is to find the mode of the surface whereas our goal is to estimate the entire surface. 356 Further, each arm in our setting corresponds to multiple instances, which gives rise to a degree of 357 heteroscedasticity and input-dependent noise that is not modeled in their settings. Lázaro-Gredilla 358 and Titsias [11], Kersting et al. [12] propose to handle heteroscedasticity by using a separate GP 359 to model the variance at each arm. However, we showed the importance of additional terms in our 360 likelihood and observation pooling to reliably represent estimation uncertainty. Wenger et al. [28] 361 propose observation pooling for estimating smooth Betas but they assume a fixed kernel. 362

Model debugging: Testing deep neural network (DNN) is another emerging area [29]. Pei et al. [30], Tian et al. [31], Sun et al. [32], Odena et al. [33] propose to generate test examples with good coverage over all activations of a DNN. Ribeiro et al. [34], Kim et al. [35] identify rules that explain the model predictions.

367 6 Conclusion

368 We presented AAA, a new approach to estimate the accuracy of a classification service, not as a single number, but as a surface over a space of attributes (arms). AAA models uncertainty with a 369 Beta distribution at each arm and regresses these parameters using two Gaussian Processes to capture 370 smoothness and generalize to unseen arms. We proposed an additional Dirichlet likelihood to mitigate 371 an over-smoothing problem with GP's estimation of Beta distributions' scale parameters. Further, to 372 protect these high-capacity GPs from unreliable accuracy observations at sparsely populated arms, 373 we propose to use an observation pooling strategy. Finally, we show how to handle noisy attribute 374 labels by an efficient joint recalibration method. Evaluation on real-life datasets and classification 375 services show the efficacy of AAA, both in estimation and exploration quality. 376

Limitation and future work: (1) We have evaluated AAA on the order of thousands of arms. Even larger attribute spaces could unearth more challenges. (2) Identifying relevant attributes for an application can be non-trivial. Future work could devise strategies for attribute selection. (3) It may be hard to characterize test-time data shifts, particularly for text — there could be subtle changes in word usage, style, or punctuation. A more expressive attribute space needs to be developed for text applications.

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477 Checklist

- 478 1. For all authors...
- (a) Do the main claims made in the abstract and introduction accurately reflect the paper's contributions and scope? [Yes]
- (b) Did you describe the limitations of your work? [Yes] In Section 6.
- (c) Did you discuss any potential negative societal impacts of your work? [N/A] We do not
 foresee any negative societal impact of our our work.
- (d) Have you read the ethics review guidelines and ensured that your paper conforms to them?[Yes]
- 486 2. If you are including theoretical results...
- (a) Did you state the full set of assumptions of all theoretical results? [N/A]

(b) Did you include complete proofs of all theoretical results? [N/A] 488 3. If you ran experiments... 489 (a) Did you include the code, data, and instructions needed to reproduce the main experimental 490 results (either in the supplemental material or as a URL)? [Yes] They are included in the 491 supplementary material. 492 (b) Did you specify all the training details (e.g., data splits, hyperparameters, how they were 493 chosen)? [Yes] They have been discussed in sufficient detail in Section 4 and more details 494 are provided in Appendix. 495 (c) Did you report error bars (e.g., with respect to the random seed after running experiments 496 multiple times)? [Yes] All our experiments are reported from multiple seeds. All our plots 497 show error bar and std. dev. for all the experiments can be found in the Appendix. 498 (d) Did you include the total amount of compute and the type of resources used (e.g., type of 499 GPUs, internal cluster, or cloud provider)? [N/A] We do not see them as relevant for our 500 paper, especially since the computation is cheap. We noted asymptotic complexity of the 501 algorithm when needed. 502 4. If you are using existing assets (e.g., code, data, models) or curating/releasing new assets... 503 (a) If your work uses existing assets, did you cite the creators? [Yes] All our datasets are publicly 504 available and are cited, noted in the Section 4. 505 (b) Did you mention the license of the assets? [Yes] The pointers to the dataset contain the 506 license 507 (c) Did you include any new assets either in the supplemental material or as a URL? [N/A] We 508 do not propose any new assets. 509 (d) Did you discuss whether and how consent was obtained from people whose data you're 510 using/curating? [N/A] 511 (e) Did you discuss whether the data you are using/curating contains personally identifiable 512 information or offensive content? [N/A] All our datasets are standard and no violations of 513 these kind have been reported on these datasets. 514 5. If you used crowdsourcing or conducted research with human subjects... 515 (a) Did you include the full text of instructions given to participants and screenshots, if applica-516 ble? [N/A] 517 (b) Did you describe any potential participant risks, with links to Institutional Review Board 518 (IRB) approvals, if applicable? [N/A] 519 (c) Did you include the estimated hourly wage paid to participants and the total amount spent on 520 participant compensation? [N/A] 521