
Evaluating multiple models using labeled and unlabeled data

Divya Shanmugam^{1*} Shuvom Sadhuka^{2*}
Manish Raghavan^{2,3} John Guttag² Bonnie Berger^{2**} Emma Pierson^{4**}

¹Cornell University

²Massachusetts Institute of Technology

⁴University of California, Berkeley

*Equal contribution, **Equal supervision

divyas@cornell.edu ssadhuka@mit.edu

Abstract

It is difficult to evaluate machine learning classifiers without large labeled datasets, which are often unavailable. In contrast, *unlabeled* data is plentiful, but not easily used for evaluation. Here, we introduce Semi-Supervised Model Evaluation (SSME), a method that uses both labeled *and* unlabeled data to evaluate machine learning classifiers. The key idea is to estimate the joint distribution of ground truth labels and classifier scores using a semi-supervised mixture model. The semi-supervised mixture model allows SSME to learn from three sources of information: unlabeled data, multiple classifiers, and probabilistic classifier scores. Once fit, the mixture model enables estimation of any metric that is a function of classifier scores and ground truth labels (e.g., accuracy or AUC). We derive theoretical bounds on the error of these estimates, showing that estimation error decreases with the number of classifiers and the amount of unlabeled data. We present experiments in four domains where obtaining large labeled datasets is often impractical: healthcare, content moderation, molecular property prediction, and text classification. Our results demonstrate that SSME estimates performance more accurately than do competing methods, reducing error by $5.1\times$ relative to using labeled data alone and $2.4\times$ relative to the next best method.

1 Introduction

Large, labeled datasets are critical for evaluation in machine learning, but such datasets are often prohibitively expensive or impossible to obtain [17, 24]. Exacerbating the challenge of evaluation, the number of off-the-shelf classifiers has increased dramatically through the widespread usage of model hubs. The modern machine learning practitioner thus has a myriad of trained models, but little labeled data with which to evaluate them.

In many domains, *unlabeled data* is much more abundant than labeled data [8, 61, 49]. To take advantage of this, we introduce Semi-Supervised Model Evaluation (SSME), a method that can be used to evaluate multiple classifiers using both labeled *and* unlabeled data. The key idea is to estimate the joint distribution of ground truth classes y and continuous classifier scores s using a mixture model, where different components of the mixture model correspond to different classes. The joint distribution allows us to evaluate performance on examples where we have access *only* to each classifier’s scores, i.e. unlabeled examples. SSME can estimate any metric that is a function of class labels and probabilistic predictions, including widely-used metrics like accuracy, expected calibration error, AUC, and AUPRC. Concretely, we can evaluate a classifier on an unlabeled point by using our estimate of $P(y, s)$.

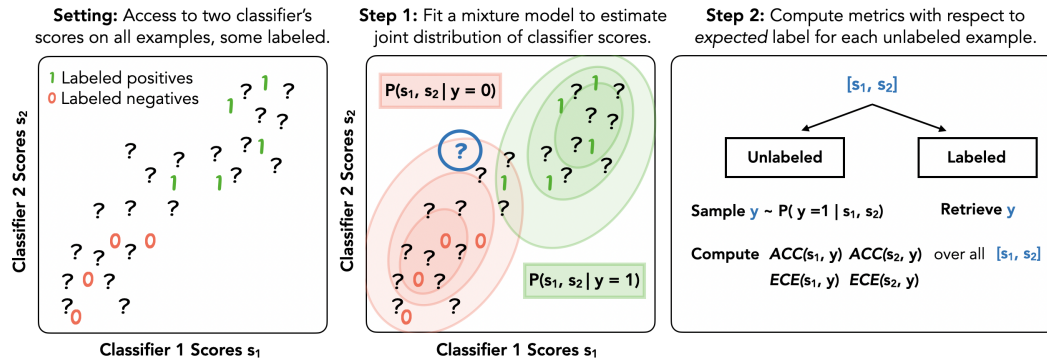


Figure 1: **Using SSME with two binary classifiers.** SSME applies to settings in which classifier scores are available for a set of examples, some labeled (left). SSME first fits a mixture model to estimate the joint density of scores and labels (where s_1 is the score assigned by the first classifier, and s_2 the second, middle panel). SSME next uses the mixture model to compute metrics with respect to the expected label for each example (right). SSME can be applied to any number of classifiers and classes K , and supports any metric that compares classifier scores to ground truth labels.

SSME is the first evaluation method to capture three key facets of modern machine learning settings: (i) multiple machine learning classifiers, (ii) probabilistic predictions over all classes, and (iii) unlabeled data. Simultaneously using all three is difficult because it requires accurately estimating the (potentially high-dimensional) joint distribution $P(y, s)$ with primarily unlabeled data. While prior work captures subsets of these three sources of information [69, 57, 37, 15, 11] — for example, augmenting labeled data with unlabeled data to evaluate a *single* classifier — no existing approach accommodates all three.

We show both theoretically and empirically that by using all available data — multiple classifiers, continuous scores over all classes, and unlabeled data — SSME is able to produce more accurate performance estimates compared to prior work. We make three contributions:

1. We propose SSME, a method that incorporates unlabeled data, continuous classifier scores, and multiple classifiers to produce more accurate performance estimates than prior work. SSME is able to estimate any metric that compares predicted probabilities to ground truth labels and accommodates varying numbers of classifiers and classes.
2. We prove that using unlabeled data and multiple classifiers improves performance estimation, providing insight into SSME’s strong empirical performance across domains.
3. We show that SSME produces more accurate performance estimates compared to labeled data alone and seven baselines, reducing metric estimation error by $5.1\times$ relative to labeled data and $2.4\times$ relative to the next best method. We further validate SSME’s utility in two case studies: evaluating large language models and subgroup-specific performance.

2 Problem Setting

We consider a setting in which a practitioner wishes to evaluate several classifiers using both labeled and unlabeled data. Formally, there are M classifiers $[f_1, f_2, \dots, f_M]$ designed for the same task, which might differ in their training data, architectures, or optimization, among other possibilities. Each classifier maps from the same input domain $\mathcal{X}$ to a probability distribution over K classes. Let $\mathbf{s}^i = [f_1(x^i), f_2(x^i), \dots, f_M(x^i)]$ denote the concatenated set of classifier scores for data point x^i ; Figure 1 depicts the setting.

We assume access to the set of classifiers and two datasets: (1) a small labeled dataset, $\mathcal{D}_L = \{(x^i, y^i)\}_{i=1}^{n_\ell}$ and (2) a larger unlabeled dataset $\mathcal{D}_U = \{(x^i)\}_{i=1}^{n_u}$. We assume that unlabeled data is far more available than labeled data, i.e. $n_u \gg n_\ell$, and that the unlabeled samples are drawn from the same distribution as the labeled samples. Our goal is to use these two datasets to estimate classifier performance using standard metrics such as expected calibration error (ECE) or accuracy. If we knew the true label y^i for each point x^i , it would be straightforward to evaluate the performance of each pre-trained classifier. However, the true label is not available for unlabeled examples, so we instead aim to infer a distribution over ground truth labels.

3 Method

Semi-supervised model evaluation (SSME) contains two key steps. First, SSME estimates the joint distribution of ground truth labels y and classifier scores $\mathbf{s}$ — i.e. $P(y, \mathbf{s})$ — using both labeled and unlabeled data. Second, SSME uses the estimate of $P(y, \mathbf{s})$ to compute metrics with respect to the posterior over y implied by classifier scores $\mathbf{s}$, allowing classifier evaluation using both labeled data (where ground truth is available) and unlabeled data (where ground truth is inferred).

Step 1: Estimating $P(y, \mathbf{s})$. SSME estimates $P(y, \mathbf{s})$ using a semi-supervised mixture model, where components of the mixture model correspond to different ground truth classes. Following standard procedures in mixture model estimation, we optimize parameters of the mixture model θ by maximizing the log-likelihood of the observed data. When y is unobserved, we treat it as a latent variable and marginalize it out. Specifically, we optimize the following expression:

$$\begin{aligned} \operatorname{argmax}_{\theta} P(\mathbf{S}, Y; \theta) &= \operatorname{argmax}_{\theta} \left[\prod_{i=1}^{n_{\ell}} P(\mathbf{s}_i, y_i; \theta) \prod_{j=1}^{n_u} P(\mathbf{s}_j; \theta)^{\lambda_U} \right] \quad (1) \\ &= \operatorname{argmax}_{\theta} \left[\underbrace{\sum_{i=1}^{n_{\ell}} \log [P_{\theta}(\mathbf{s}_i | y_i) P_{\theta}(y_i)]}_{\text{Labeled Data Log-Likelihood}} + \lambda_U \underbrace{\sum_{j=1}^{n_u} \log \sum_{k=1}^K [P_{\theta}(\mathbf{s}_j | y_j = k) P_{\theta}(y_j = k)]}_{\text{Unlabeled Data Log-Likelihood}} \right] \quad (2) \end{aligned}$$

where λ_U controls the relative weight of the unlabeled data in the likelihood; we fix $\lambda_U = 1$.

We optimize the above expression using expectation-maximization (EM) [19, 76], alternating between the E-step, which estimates which mixture component (i.e. ground truth class) each data point belongs to, and the M-step, which estimates the parameters of each component based on the soft component assignments. Algorithm 1 details the EM procedure we use to fit our mixture model.

A technical challenge when fitting densities on bounded domains, as is the case with classifier outputs, is *boundary bias*, where estimates of density are biased near edges of the domain [39]. To overcome this challenge, we transform probabilistic predictions over K classes to points (“scores”) in $\mathbb{R}^{K-1}$ using the additive log-ratio transform, which produces a one-to-one mapping between the two spaces [1, 53]. Additive log-ratio transforms are a *reparameterization trick*: they transform the classifier scores from a hard-to-model space — the probability simplex — to an easier-to-model space — unbounded reals. Appendix E.1 provides the expression for the additive log-ratio transform.

Step 2: Estimating classifier performance given $P(y, \mathbf{s})$. Once we have estimated the parameters θ for the mixture model, we can use the fitted density to estimate metrics of interest, using the procedure described in Figure 1. By estimating the conditional distribution $P_{\theta}(y | \mathbf{s})$, SSME can measure performance with respect to the *expected* label of unlabeled examples (where we observe only $\mathbf{s}^i$). Specifically, we sample ground truth labels y from the distribution $P_{\theta}(y | \mathbf{s})$ for all unlabeled examples. Labeled examples retain their ground truth labels. We then compute metrics with respect to both the sampled and ground truth labels, and average the estimated metric across samples. SSME can estimate any metric that is a function of classifier scores and ground truth labels; see Algorithm 2 for corresponding pseudocode.

The proposed approach enjoys several properties. By using a semi-supervised mixture model, SSME takes advantage of unlabeled data to estimate $P(y, \mathbf{s})$. SSME also naturally accommodates and benefits from additional classifiers, because they can provide additional information about the ground truth label of an unlabeled example (additional classifiers simply translate to additional dimensions in $\mathbf{s}$). Furthermore, the use of the additive log-ratio transform allows SSME to learn directly from continuous class probabilities for each input, as opposed to discretized labels.

3.1 Implementation

SSME can accommodate multiple ways to parametrize the class-conditional distribution of scores $P(\mathbf{s} | y)$ as long as they can be learned in the semi-supervised setting described above. We denote the parameterized distribution as $P_{\theta}(\mathbf{s} | y)$. In our experiments, we use a kernel density estimator (KDE) to parameterize $P_{\theta}(\mathbf{s} | y)$ and explore alternative parametrizations of $P(\mathbf{s}^{(i)} | y^{(i)})$ in Appendix E.3.

Algorithm 1: Estimating $P(y, \mathbf{s})$ using EM

Input: Labeled set $\mathcal{D}_\ell = \{(\mathbf{s}^i, y^i)\}_{i=1}^{n_\ell}$; Unlabeled set $\mathcal{D}_u = \{\mathbf{s}^i\}_{i=1}^{n_u}$; $\mathbf{s}^i$ are ALR-transformed classifier scores; Labeled-data weight λ_U ; number of classes K ; total epochs $T = 1000$

Init: Initialize model parameters θ^0 ;
Initialize class priors $p^0(y = k) = \hat{p}(y = k)$; // empirical class distribution

```
1 for  $t \leftarrow 0$  to  $T - 1$  do
2   E-step: compute responsibilities  $\gamma_{ik}$ ;
3   foreach  $\mathbf{s}^{(i)} \in \mathcal{D}_u$  do
4     for  $k \leftarrow 1$  to  $K$  do
5        $\gamma_{ik} \leftarrow \frac{p^t(y = k) P_{\theta^t}(\mathbf{s}^{(i)} | y = k)}{\sum_{\ell=1}^K p^t(y = \ell) P_{\theta^t}(\mathbf{s}^{(i)} | y = \ell)}$ ;
6   foreach  $(\mathbf{s}^i, y^i) \in \mathcal{D}_\ell$  do
7      $\gamma_{ik} \leftarrow \mathbf{1}[k = y^i]$ ; // fix to true label
8   M-step: update priors and  $\theta$ ;
9   for  $k \leftarrow 1$  to  $K$  do
10     $N_k \leftarrow \sum_{\mathcal{D}_u} \gamma_{ik} + \lambda_U \sum_{\mathcal{D}_\ell} \gamma_{ik}$ ; // weighted effective count for class  $k$ 
11     $p^{t+1}(y = k) \leftarrow N_k / (n_u + \lambda_U n_\ell)$ ;
12     $\theta^{t+1} \leftarrow \arg \max_{\theta} \sum_{i=1}^{n_u+n_\ell} w_i \sum_{k=1}^K \gamma_{ik} \log P_{\theta}(\mathbf{s}^i | y = k)$ ,
13    where  $w_i = \lambda_U$  for unlabeled points and  $w_i = 1$  otherwise;
```

Output: Final parameters θ^T and priors $p^T(y)$

Kernel density estimators do not make parametric assumptions about the distributional form of each component: this is useful for modeling distributions of predictions, which can vary widely across tasks and classifiers. The KDE for the k th class is parametrized by bandwidth h and the kernel type $\mathcal{K}$. We weight each point by the probability it belongs to the component (i.e., a soft label). When $\mathbf{s}^i$ is labeled, $P(y^i = k) = 1$ for the true label k , and when $\mathbf{s}^i$ is unlabeled, we compute $P(y^i = k | \mathbf{s})$ using the estimated density. For all experiments, we fit use a Gaussian kernel and estimate h using the improved Sheather-Jones algorithm [10]. We optimize the parameters using EM over 1000 epochs. We initialize component assignments by drawing a label for a given example according to the mean classifier score across the set of classifiers.

3.2 Theoretical analysis

We motivate our approach by deriving bounds for how well a semi-supervised estimation procedure can estimate classifier performance in a setting where classifier scores $\mathbf{s}$ are drawn from a mixture of Gaussians.

Model of y and $\mathbf{s}$. We consider a stylized binary classification setting drawn from previous work [67] where classifier scores $\mathbf{s}$ are drawn from a balanced mixture of two Gaussians. For data in the positive class, classifier scores are drawn from a multivariate Gaussian $\mathcal{N}(c, I)$. For data in the negative class, classifier scores are drawn from a multivariate Gaussian $\mathcal{N}(0, I)$. Let n_u refer to the number of unlabeled examples, n_ℓ the number of labeled examples, and d the number of classifiers. Additional classifiers increase the dimensionality of the multivariate Gaussian.

Performance estimation procedure. Having specified how classifier scores are generated, we analyze how accurately a semi-supervised performance estimation procedure similar to our own can estimate classifier performance. We consider a class of semi-supervised learning algorithms frequently analyzed in prior work, UL+ [67]. UL+ algorithms first use the unlabeled data to identify decision boundaries and then use the labeled data to assign regions to classes. AUC_k and ACC_k represent ground truth performance of classifier k ; $\widehat{AUC}_k$ and $\widehat{ACC}_k$ are performance estimators that use UL+ to estimate a Gaussian mixture model, and use that model to estimate performance. We apply bounds developed by [67] for errors in mixture model estimation to bound errors in performance estimation.

Theorem 1 Let $\widehat{AUC}_k, \widehat{ACC}_k$ be estimated using a semi-supervised learning algorithm in the UL+ class of estimators. When $n_u \gtrsim \max \left\{ d, \frac{d}{\|c\|^4}, \frac{\log(n_u)}{\min\{\|c\|^2, \|c\|^4\}}, \frac{d \log(d n_u)}{\|c\|^6} \right\}$ and $d \geq 2$, the following bounds on error in estimated performance hold with probability $1 - p$:

$$|AUC_k - \widehat{AUC}_k| \leq \Phi\left(\frac{\mathbf{c}_k}{\sqrt{2}}\right) - \Phi\left(\frac{\mathbf{c}_k - \epsilon_c}{\sqrt{2}}\right) \quad (3)$$

$$|ACC_k - \widehat{ACC}_k| \leq \Phi\left(\frac{\mathbf{c}_k}{2}\right) - \Phi\left(\frac{\mathbf{c}_k - \epsilon_c}{2}\right) \quad (4)$$

where $\epsilon_c \lesssim \frac{1}{p} \left(\sqrt{\frac{d}{\|c\|^2 n_u}} + \|c\| e^{-\frac{1}{2} n_l \|c\|^2} \left(1 - \frac{C_0}{\|c\|^2} \sqrt{\frac{d \log(n_u)}{\|c\|^2 n_u}} \right)^2 \right)$ and C_0 is a universal constant.

The expression for ϵ_c captures its asymptotic dependence on n_u, n_l, d , and c . Smaller ϵ_c correspond to smaller errors in performance estimation. Section C contains the full proof, which consists of two steps: we first bound the error in estimating the separation of the two Gaussian components $\|c\|$, and then use the relationship between component separation and classifier performance to bound error in estimates of AUC and accuracy.

Analysis. Our theoretical bounds have several implications. First, unlabeled data helps: increases in n_u reduce both the first term and the second term. This indicates why SSME outperforms baselines that only make use of labeled data: additional unlabeled data improves our ability to accurately estimate components of a mixture model ($\epsilon_c \approx O(1/\sqrt{n_u})$). Second, bounds tighten as separation between components $\|c\|$ grows, i.e. when classifiers in the set are more accurate. Third, bounds tighten as the number of classifiers increases, so long as the increase in separation $\|c\|$ outweighs the cost of an additional dimension in d ; we precisely characterize this setting in Section C.1. This helps explain why SSME outperforms work that makes use of a single classifier, instead of several.

Our theoretical results are derived for a stylized setting frequently studied in prior work [59, 60, 67, 26]. While this setting differs from our empirical setting – for example, it uses a simplified semi-supervised learning algorithm – we verify that trends our theory implies hold robustly in both synthetic and real experiments (Sec. 5, D.1), including settings where these assumptions do not hold.

4 Experiments

4.1 Datasets and Classifier Sets

We select datasets and classifier sets to be realistic and diverse, capturing multiple modalities (EHRs, text, and graphs), domains (healthcare, content moderation, chemistry), and architectures (logistic regressions, graph neural networks, large language models). We report ground truth metrics for the binary and multiclass classifiers in Tables S1 and S2 respectively. We also include a detailed description of each dataset and classifier set in Appendix B.1. We summarize each dataset and differences between classifiers in the associated classifier set below.

We evaluate SSME on five classification datasets: (1) **MIMIC-IV** [38], a dataset of Boston-area electronic health records (EHRs) with three hospitalization outcomes (critical outcome, ED revisit within 30 days, and hospital admission) with classifiers drawn from prior works [50]; (2) **Civil-Comments** [9], a dataset of social media comments flagged as “toxic” or not by human annotators, with pretrained classifiers downloaded from the WILDS benchmark [42]; (3) **OGB-SARS-CoV** [33], a molecular property prediction task, with pretrained classifiers downloaded from WILDS; (4) **MultiNLI**, a natural language task, with classifiers drawn from the SubpopBench dataset [73]; and (5) **AG News** [75], a news classification task, using open-source and closed-source LLMs as classifiers.

4.2 Baselines

We compare SSME to eight baselines that use both labeled and unlabeled data to estimate performance (with the exception of **Labeled**, the standard approach to classifier evaluation, which only uses examples for which labels are available). The remaining baselines cover a broad range of approaches one could adapt to semi-supervised evaluation and fall into three categories. For a full description of each baseline’s implementation, please refer to Appendix B.2.

The first category fits a model of $P(y, \mathbf{s})$ using labeled data alone, then applies it to the entire dataset. Each baseline does so in a different way: Pseudo-Labeled (**PL**) fits a logistic regression to predict the true label from classifier scores; Bayesian-Calibration (**BC**) [37] fits a Bayesian model to re-calibrate each classifier's predicted probabilities; **AutoEval** [11] learns a function to debias classifier predictions. The second category estimates the performance of individual classifiers. **SPE** [69] fits a parametric mixture model to a single classifier's predictions. **Active-Testing** [44] uses active learning to select examples to label out of a pool of unlabeled examples based on a single classifier's predictions and evaluates the classifier on those examples. The last category of baselines is drawn from the multiple annotator literature, where annotations are assumed to be discrete. We compare to **Dawid-Skene** [18], which accepts discrete annotations from each classifier to estimate the latent true label for each example. We also compare to **Majority-Vote**, which ensembles classifier predictions by performing an accuracy-weighted aggregation of classifier predictions.

We also provide a comparison to completely unsupervised approaches (including ensembling where the "ground truth" label is drawn based on the average classifier score) in Sec. D.10, and discuss connections to weak supervision in Sec. D.9.

4.3 Evaluation

We evaluate SSME's ability to estimate four performance metrics for binary classifiers: accuracy, area under the receiver operating characteristic curve (AUC), area under the precision-recall curve (AUPRC), and the expected calibration error (ECE). For multi-class problems, we evaluate accuracy and top-label calibration error [32].

We partition each dataset into three splits: the classifier training split (used to train the classifiers whose performance SSME estimates), the estimation split (used to fit SSME and estimate classifier performance), and the evaluation split (used to produce a held-out, ground-truth measure of classifier performance). All splits are sampled from the same distribution, except when estimating subgroup-specific performance, where the evaluation split contains a subset of the test distribution.

To evaluate metric estimates, we measure the absolute error of the *estimated* metric, computed using the estimation split, compared to the *true* metric, computed on the held-out evaluation split (averaging over classifiers in the set). The estimation split consists of either 20, 50, or 100 labeled examples and 1000 unlabeled examples across all experiments. The size of the evaluation split is on the order of thousands of labeled examples and varies by task (see Appendix B.1 for exact split sizes). To quantify uncertainty, we compute 95% confidence intervals using the standard error of the mean across 50 random data splits ($\pm 1.96 \times \text{SEM}$). In line with prior work, we report rescaled estimation error for each metric (where errors are relative to using labeled data alone), allowing us to standardize the scale of errors across datasets and metrics [28].

5 Results

5.1 SSME produces more accurate performance estimates than prior work

We now compare SSME to eight baselines in terms of its ability to estimate classifier performance on five binary tasks. All figures report rescaled metric estimation error (RMAE; lower is better) and reflect performance estimation using 20 labeled examples and 1000 unlabeled examples. Results are consistent across additional values of n_ℓ (50 and 100; see results in D.2), although labeled data grows more competitive (as expected) with larger labeled dataset sizes.

Comparison to baselines SSME achieves lower mean estimation error (averaging across tasks and metrics) than all baselines, indicating more accurate estimation of classifier performance. SSME reduces estimation error by $5.1\times$ relative to labeled data alone (averaged across tasks and metrics). In contrast, the next best method reduces estimation error by $2.4\times$. SSME also outperforms baselines on specific metrics. For accuracy, SSME reduces metric estimation error, relative to using labeled data alone, by $5.6\times$ (averaged across tasks); the next best method for each dataset reduces metric estimation error by $2.0\times$. While the magnitude by which SSME beats baselines varies—for example, SSME reduces error by $2.9\times$ on AUC (averaged across tasks), while the next best method reduces error by $2.6\times$ —SSME consistently outperforms baselines across metrics. SSME performs on par with or better than the strongest baseline in 51 of 60 dataset, metric, and labeled data combinations

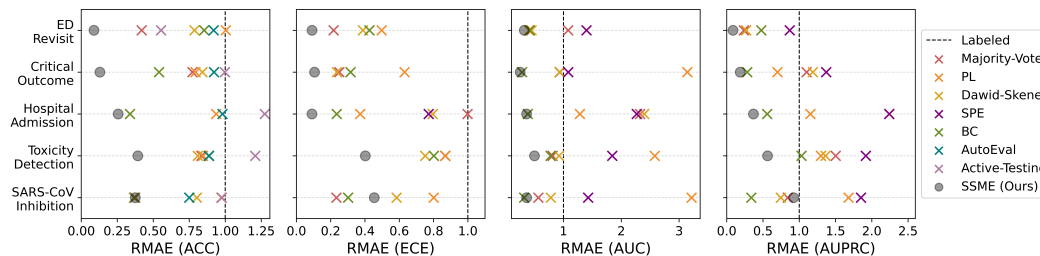


Figure 2: **Metric estimation error on binary tasks ($n_\ell = 20$, $n_u = 1000$).** Each point plots the rescaled mean absolute error (RMAE) across runs, where 1.0 (dashed line) represents the RMAE when using labeled data alone and lower is better. SSME (gray) achieves lower estimation error than the baselines, averaging across metrics and 50 runs, reported for five binary tasks (y-axis). Results reporting mean absolute error (unscaled) and 95% CIs are in Tables S3-S6.

we study, and significantly better in 31 settings (Tables S3-S6). Figure 2 summarizes how SSME compares to several baselines across various metrics and tasks¹.

Our results are also encouraging in absolute terms. With 20 labeled examples and 1000 unlabeled examples, SSME estimates accuracy within 1.5 percentage points (averaging across tasks). The closest baseline estimates accuracy within 3.4 percentage points. Results comparing SSME to the next best baseline on other metrics (1.9 vs 3.8 on ECE; 3.6 vs 4.3 on AUC; 8.5 vs 10.2 on AUPRC) confirm that SSME not only achieves more accurate classifier performance estimation compared to prior work, but that the resulting performance estimates are reasonably close to the ground truth.

Consistent with our theoretical results, SSME estimates performance more accurately because it makes use of all available information: multiple classifiers, continuous scores over all classes, and unlabeled data. *Dawid-Skene* and *AutoEval* discretize classifier scores (although *AutoEval* does make use of classifier confidence associated with each discrete prediction). *Pseudo-Labeling*, *Bayesian-Calibration*, and *AutoEval* each learn a mapping from s to y using only the labeled data and apply that mapping to the unlabeled data (rather than learning from labeled and unlabeled data together). By jointly learning across both labeled and unlabeled data, SSME is able to generalize much better in cases where there aren't enough labels to estimate the joint distribution of classifier scores and labels from labeled examples alone. Finally, *Bayesian-Calibration* and *SPE* learn from a single classifier's scores, and do not learn from multiple classifiers at once.

Comparison across metrics SSME provides the greatest benefits relative to labeled data alone when measuring expected calibration error (ECE), with a reduction in estimation error of $7.2\times$ (averaging across tasks). ECE is harder to estimate with few labeled examples because it requires binning and then averaging calibration error across bins, producing greater variability when the number of labeled points per bin is small. We observe the smallest benefits relative to labeled data alone when measuring AUPRC (a reduction in estimation error of $2.2\times$, relative to labeled data).

Comparison across amounts of labeled data SSME's performance continues to improve with more labeled data, but the advantage it confers over labeled data alone decreases: for example, with 20, 50, and 100 datapoints, SSME outperforms labeled data alone by $5.6\times$, $3.0\times$, and $1.6\times$. Similar to labeled data alone, there are diminishing but positive returns to adding labeled data to SSME's performance estimation procedure.

Another way to quantify SSME's benefit is to measure the amount of labeled data required to match SSME's performance, or the *effective sample size* (ESS), as introduced by prior work [11] (see Appendix B.3 for implementation details). With access to 20 labeled examples and 1000 unlabeled examples, SSME achieves an average ESS of 539 labeled examples for estimating ECE (averaging over tasks). In contrast, the next best approach achieves an ESS of 110 labeled examples.

Comparison to marginal fit To validate the benefit of fitting the mixture model to multiple classifiers simultaneously, we compare to an ablated version of SSME fit on a single classifier at a time, SSME-M. SSME-M estimates the classifier-specific marginal distribution of $P(y|s)$, and uses

¹Fig. 2 omits results for Dawid-Skene (accuracy) and Majority-Vote (accuracy) on hospital admission, and SPE (ECE) because their higher RMAEs distort the plotting scale. Tables S3 - S6 contain complete results across baselines, including uncertainty estimates.

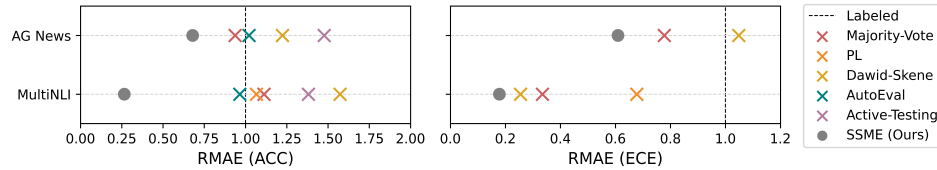


Figure 3: **Metric estimation error for LLM classifiers ($n_\ell = 20$, $n_u = 1000$).** SSME consistently reduces estimation error relative to labeled data alone and does so more reliably than any baseline capable of estimating performance in multiclass settings.

this estimate to evaluate the classifier in question. Doing so results in worse performance estimates across metrics, tasks, and amounts of labeled data (Tables S3- S6) relative to our full model. This agrees with our theoretical findings: each classifier provides distinct information about the ground truth label for a given example, which SSME is able to use.

Supplementary results The supplement contains additional results. We report mean absolute error, including standard errors and additional n_ℓ , for accuracy, ECE, AUC, and AUPRC in Tables S3- S6 (broken down by classifier in Tables S7- S10). We report the sensitivity of SSME to kernel choice in Table S13. Section D.11 provides a computational cost analysis of SSME relative to the baselines. Finally, we provide synthetic experiments to substantiate our theoretical findings under violations of our assumptions in Section D.1.

5.2 Case study: Evaluating classifiers derived from large language models

Large language models (LLMs) are increasingly used to create classifiers [40, 66, 68], with demonstrated potential to serve as data annotators [78]. However, evaluation of LLM-based classifiers is limited by the availability of labeled data. We study SSME’s ability to estimate performance in this setting.

We evaluate classifiers derived from large language models on the MultiNLI and AG News datasets: the MultiNLI classifier set contains off-the-shelf language model based classifiers, while the AG News classifier set contains four classifiers trained atop open- and closed-source large language models. Fig. 3 reports our results. We find that SSME improves over labeled data by $2.3\times$ (averaging over tasks and metrics). In contrast, the next best baseline (Majority-Vote) improves over labeled data by $1.3\times$. SSME achieves significantly lower metric estimation error in 8 of the 12 combinations of task, metric, and n_ℓ , and performs comparably to the next best baseline in 3 of the remaining 4 combinations (Tables S11, S12).

	Age	Sex	Race
PL	0.92	1.06	1.13
Dawid-Skene	0.75	0.67	0.67
BC	0.45	0.33	0.41
SSME (Ours)	0.42	0.19	0.39

Table 1: **Subgroup-specific performance estimation ($n_l = 20$, $n_u = 1000$).** SSME achieves the lowest rescaled metric estimation error (RMAE), averaging across metrics and subgroups.

5.3 Case study: Evaluating subgroup-specific performance

SSME can be applied to measure performance within demographic subgroups, a task central to assessments of algorithmic fairness [12]. We conduct our analysis in the context of critical outcome prediction on MIMIC-IV, a task with documented prediction disparities [50], and a set of commonly studied demographic groups (age, sex, race/ethnicity). We produce subgroup-specific performance estimates by sampling ground truth labels y according to our estimated $p(y|s)$ for only those s observed among a given demographic group. We perform this analysis with respect to demographic groups based on age, sex, and race/ethnicity. When there is no labeled data for a given subgroup, *Labeled* estimates subgroup-specific performance as global performance.

We report each method’s reduction in estimation error relative to labeled data (averaging over metrics and subgroups) for each demographic category in Table 1, comparing to all baselines that can estimate the four performance metrics we average over. SSME reduces metric estimation error by $5.3\times$ on sex, $2.6\times$ on race, and $2.4\times$ on age relative to labeled data, and to a greater extent than all baselines. SSME outperforms all baselines on all individual metrics except for AUC, for which BC reduces estimation error by $3.2\times$ as compared to $2.2\times$ for SSME. BC is well-suited to estimating AUC because it assumes monotonicity when mapping s to y ; i.e., $P(y = 1|s^{(i)}) \geq P(y = 1|s^{(j)})$ when

$s^{(i)} \geq s^{(j)}$. When the classifiers in question have high AUCs — as the critical outcome classifiers do — this is a useful assumption.

6 Related Work

Our work unifies ideas from two literatures: methods to 1) evaluate a single classifier and 2) evaluate the accuracy of multiple discrete annotators in the presence of labeled and unlabeled data.

Classifier evaluation is a long-standing problem in machine learning. Early work on the use of unlabeled data for classifier evaluation made progress via assumptions about the available unlabeled data (for example, assumptions about class priors [6, 23, 47]; conditionally independent features [64]; well-calibrated classifiers [30]; models of covariate shift [13, 45]). SSME avoids such assumptions by using both labeled and unlabeled data to learn a flexible semi-supervised mixture model of classifier predictions. Interest in unsupervised evaluation has surged in the context of large language models, where models are often judged by other models [77, 34]. These approaches, while promising, are tailored to text generation and not applicable to broader classification tasks. A parallel line of work aims to make use of both labeled and unlabeled data to estimate classifier performance. Existing methods operate on individual classifiers and assume specific parametric forms for the prediction distributions [69, 15, 36, 37, 25]. Some works also focus on model selection in semi-supervised settings, though they do not explicitly estimate performance [46]. SSME differs from these works by naturally capitalizing on multiple classifiers, continuous classifier scores, and unlabeled data. As our results show, doing so leads to improved estimates of performance.

Evaluation of multiple discrete annotators was first introduced by [18], who proposed a method to estimate ground truth in the presence of multiple potentially noisy discrete annotations. Many subsequent works inherit Dawid-Skene’s strong assumption of class-conditional independence of annotator errors [52, 57], including popular approaches in weak supervision [58, 4, 27], where annotators are instead user-provided labeling functions. Such an assumption is plausible in certain contexts, but does not naturally translate to sets of candidate classifiers, whose predictions are likely to be correlated. However, methods from this line of work are designed to estimate the accuracy of *binary* annotations; they do not exploit the continuous probabilities available in multi-classifier evaluation. While some work has made progress towards accommodating continuous predicted probabilities [51, 56], their focus is optimal aggregation, in contrast to our own, which is evaluation. Recent works use a continuous notion of classifier confidence in conjunction with discrete annotations from each annotator [29, 11], but do not use the distribution of classifier scores over *all* classes.

7 Discussion

In this paper, we presented Semi-Supervised Model Evaluation (SSME), a method that supplements limited labeled data with *unlabeled data* to more accurately estimate classifier performance. SSME leverages three features of the current machine learning landscape: (i) there are frequently multiple classifiers for the same task, (ii) continuous classifier scores are often available for all classes, and (iii) unlabeled data is often far more plentiful than labeled data. We provide theoretical bounds on performance estimation error that help explain SSME’s advantages over prior work. We show that across multiple tasks, architectures, and modalities, SSME substantially outperforms using labeled data alone and standard baselines.

Our results, and their accompanying limitations, suggest several directions for future work. First, each of the metrics we examined (e.g., AUC) evaluate a single classifier. But because SSME estimates the full joint distribution $P(y, \mathbf{s})$, it could be used to measure properties of the classifiers as a set. For instance, recent work has highlighted the importance of measuring *algorithmic monoculture* [41] where all classifiers produce errors on the same instances. Second, our experiments assess settings in which the unlabeled data is sampled from the same distribution as the labeled data. Although this is common — for example, when a random subset of examples is annotated — many real-world scenarios violate this assumption, and extending SSME to settings with such distribution shift represents an important next step [61]. Finally, our current implementation relies on kernel density estimation, which can scale poorly in high-dimensional spaces (e.g., with many classifiers or classes). Exploring more scalable density estimators could further broaden SSME’s applicability. More generally, our results indicate that SSME offers a principled and practical framework for accurate performance estimation in the absence of a large labeled dataset.

References

- [1] John Aitchison. The statistical analysis of compositional data. *Journal of the Royal Statistical Society: Series B (Methodological)*, 44(2):139–160, 1982.
- [2] Michael S Albergo and Eric Vanden-Eijnden. Building normalizing flows with stochastic interpolants. *arXiv preprint arXiv:2209.15571*, 2022.
- [3] Anastasios N Angelopoulos, Stephen Bates, Clara Fannjiang, Michael I Jordan, and Tijana Zrnica. Prediction-powered inference. *Science*, 382(6671):669–674, 2023.
- [4] Stephen H Bach, Bryan He, Alexander Ratner, and Christopher Ré. Learning the structure of generative models without labeled data. In *International Conference on Machine Learning*, pages 273–282. PMLR, 2017.
- [5] Christina Baek, Yiding Jiang, Aditi Raghunathan, and J Zico Kolter. Agreement-on-the-line: Predicting the performance of neural networks under distribution shift. *Advances in Neural Information Processing Systems*, 35:19274–19289, 2022.
- [6] Krishnakumar Balasubramanian, Pinar Donmez, and Guy Lebanon. Unsupervised supervised learning ii: Margin-based classification without labels. In *Proceedings of the Fourteenth International Conference on Artificial Intelligence and Statistics*, pages 137–145. JMLR Workshop and Conference Proceedings, 2011.
- [7] Barry Becker and Ronny Kohavi. Adult. UCI Machine Learning Repository, 1996. DOI: <https://doi.org/10.24432/C5XW20>.
- [8] Tristan Bepler, Andrew Morin, Micah Rapp, Julia Brasch, Lawrence Shapiro, Alex J Noble, and Bonnie Berger. Positive-unlabeled convolutional neural networks for particle picking in cryo-electron micrographs. *Nature methods*, 16(11):1153–1160, 2019.
- [9] Daniel Borkan, Lucas Dixon, Jeffrey Sorensen, Nithum Thain, and Lucy Vasserman. Nuanced metrics for measuring unintended bias with real data for text classification. In *Companion proceedings of the 2019 world wide web conference*, pages 491–500, 2019.
- [10] ZI Botev, JF Grotowski, and DP Kroese. Kernel density estimation via diffusion. *Annals of Statistics*, 38(5):2916–2957, 2010.
- [11] Pierre Boyeau, Anastasios N Angelopoulos, Nir Yosef, Jitendra Malik, and Michael I Jordan. Autoeval done right: Using synthetic data for model evaluation. *arXiv preprint arXiv:2403.07008*, 2024.
- [12] Irene Y Chen, Emma Pierson, Sherri Rose, Shalmali Joshi, Kadija Ferryman, and Marzyeh Ghassemi. Ethical machine learning in healthcare. *Annual review of biomedical data science*, 4(1):123–144, 2021.
- [13] Lingjiao Chen, Matei Zaharia, and James Y Zou. Estimating and explaining model performance when both covariates and labels shift. *Advances in Neural Information Processing Systems*, 35:11467–11479, 2022.
- [14] Victor Chernozhukov, Denis Chetverikov, Mert Demirer, Esther Duflo, Christian Hansen, Whitney Newey, and James Robins. Double/debiased machine learning for treatment and structural parameters, 2018.
- [15] Alexandra Chouldechova, Siqi Deng, Yongxin Wang, Wei Xia, and Pietro Perona. Unsupervised and Semi-supervised Bias Benchmarking in Face Recognition. In Shai Avidan, Gabriel Brostow, Moustapha Cissé, Giovanni Maria Farinella, and Tal Hassner, editors, *Computer Vision – ECCV 2022*, Lecture Notes in Computer Science, pages 289–306, Cham, 2022. Springer Nature Switzerland.
- [16] Rob Cornish, Anthony Caterini, George Deligiannidis, and Arnaud Doucet. Relaxing bijectivity constraints with continuously indexed normalising flows. In *International conference on machine learning*, pages 2133–2143. PMLR, 2020.

- [17] Aron Culotta and Andrew McCallum. Reducing labeling effort for structured prediction tasks. In *AAAI*, volume 5, pages 746–751, 2005.
- [18] Alexander Philip Dawid and Allan M Skene. Maximum likelihood estimation of observer error-rates using the em algorithm. *Journal of the Royal Statistical Society: Series C (Applied Statistics)*, 28(1):20–28, 1979.
- [19] Arthur P Dempster, Nan M Laird, and Donald B Rubin. Maximum likelihood from incomplete data via the EM algorithm. *Journal of the royal statistical society: series B (methodological)*, 39(1):1–22, 1977.
- [20] Weijian Deng, Yumin Suh, Stephen Gould, and Liang Zheng. Confidence and dispersity speak: Characterizing prediction matrix for unsupervised accuracy estimation. In *International Conference on Machine Learning*, pages 7658–7674. PMLR, 2023.
- [21] Weijian Deng and Liang Zheng. Are labels always necessary for classifier accuracy evaluation? In *Proceedings of the IEEE/CVF conference on computer vision and pattern recognition*, pages 15069–15078, 2021.
- [22] Laurent Dinh, Jascha Sohl-Dickstein, and Samy Bengio. Density estimation using real NVP. *arXiv preprint arXiv:1605.08803*, 2016.
- [23] Pinar Donmez, Guy Lebanon, and Krishnakumar Balasubramanian. Unsupervised Supervised Learning I: Estimating Classification and Regression Errors without Labels. 2010.
- [24] Suparna Dutta and Monidipa Das. Remote sensing scene classification under scarcity of labelled samples—a survey of the state-of-the-arts. *Computers & Geosciences*, 171:105295, 2023.
- [25] Vasilii Feofanov, Malik Tiomoko, and Aladin Virmaux. Random matrix analysis to balance between supervised and unsupervised learning under the low density separation assumption. In *International Conference on Machine Learning*, pages 10008–10033. PMLR, 2023.
- [26] Spencer Frei, Difan Zou, Zixiang Chen, and Quanquan Gu. Self-training converts weak learners to strong learners in mixture models. In *International Conference on Artificial Intelligence and Statistics*, pages 8003–8021. PMLR, 2022.
- [27] Daniel Fu, Mayee Chen, Frederic Sala, Sarah Hooper, Kayvon Fatahalian, and Christopher Ré. Fast and three-rious: Speeding up weak supervision with triplet methods. In *International conference on machine learning*, pages 3280–3291. PMLR, 2020.
- [28] Saurabh Garg, Sivaraman Balakrishnan, Zachary C Lipton, Behnam Neyshabur, and Hanie Sedghi. Leveraging unlabeled data to predict out-of-distribution performance. *arXiv preprint arXiv:2201.04234*, 2022.
- [29] Hui Wen Goh, Ulyana Tkachenko, and Jonas Mueller. Crowdlab: Supervised learning to infer consensus labels and quality scores for data with multiple annotators. *arXiv preprint arXiv:2210.06812*, 2022.
- [30] Devin Guillory, Vaishaal Shankar, Sayna Ebrahimi, Trevor Darrell, and Ludwig Schmidt. Predicting with confidence on unseen distributions. In *Proceedings of the IEEE/CVF international conference on computer vision*, pages 1134–1144, 2021.
- [31] Chuan Guo, Geoff Pleiss, Yu Sun, and Kilian Q Weinberger. On calibration of modern neural networks. In *International conference on machine learning*, pages 1321–1330. PMLR, 2017.
- [32] Chirag Gupta and Aaditya Ramdas. Top-label calibration and multiclass-to-binary reductions. In *International Conference on Learning Representations*, 2022.
- [33] Weihua Hu, Matthias Fey, Marinka Zitnik, Yuxiao Dong, Hongyu Ren, Bowen Liu, Michele Catasta, and Jure Leskovec. Open graph benchmark: Datasets for machine learning on graphs. *Advances in neural information processing systems*, 33:22118–22133, 2020.
- [34] Hui Huang, Yingqi Qu, Jing Liu, Muyun Yang, and Tiejun Zhao. An empirical study of llm-as-a-judge for llm evaluation: Fine-tuned judge models are task-specific classifiers. *arXiv preprint arXiv:2403.02839*, 2024.

- [35] Pavel Izmailov, Polina Kirichenko, Marc Finzi, and Andrew Gordon Wilson. Semi-supervised learning with normalizing flows. In *International conference on machine learning*, pages 4615–4630. PMLR, 2020.
- [36] Disi Ji, Robert L Logan, Padhraic Smyth, and Mark Steyvers. Active bayesian assessment of black-box classifiers. In *Proceedings of the AAAI Conference on Artificial Intelligence*, volume 35, pages 7935–7944, 2021.
- [37] Disi Ji, Padhraic Smyth, and Mark Steyvers. Can i trust my fairness metric? assessing fairness with unlabeled data and bayesian inference. *Advances in Neural Information Processing Systems*, 33:18600–18612, 2020.
- [38] Alistair Johnson, Lucas Bulgarelli, Tom Pollard, Steven Horng, Leo Anthony Celi, and Roger Mark. Mimic-iv. *PhysioNet*. Available online at: [https://physionet.org/content/mimiciv/1.0/\(accessed August 23, 2021\)](https://physionet.org/content/mimiciv/1.0/(accessed August 23, 2021)), pages 49–55, 2020.
- [39] M Chris Jones. Simple boundary correction for kernel density estimation. *Statistics and computing*, 3:135–146, 1993.
- [40] Neel Kant, Raul Puri, Nikolai Yakovenko, and Bryan Catanzaro. Practical text classification with large pre-trained language models. *arXiv preprint arXiv:1812.01207*, 2018.
- [41] Jon Kleinberg and Manish Raghavan. Algorithmic monoculture and social welfare. *Proceedings of the National Academy of Sciences*, 118(22):e2018340118, 2021.
- [42] Pang Wei Koh, Shiori Sagawa, Henrik Marklund, Sang Michael Xie, Marvin Zhang, Akshay Balsubramani, Weihua Hu, Michihiro Yasunaga, Richard Lanus Phillips, Irena Gao, et al. Wilds: A benchmark of in-the-wild distribution shifts. In *International conference on machine learning*, pages 5637–5664. PMLR, 2021.
- [43] Jannik Kossen, Sebastian Farquhar, Yarin Gal, and Thomas Rainforth. Active surrogate estimators: An active learning approach to label-efficient model evaluation. *Advances in Neural Information Processing Systems*, 35:24557–24570, 2022.
- [44] Jannik Kossen, Sebastian Farquhar, Yarin Gal, and Tom Rainforth. Active testing: Sample-efficient model evaluation. In *International Conference on Machine Learning*, pages 5753–5763. PMLR, 2021.
- [45] JoonHo Lee, Jae Oh Woo, Hankyu Moon, and Kwonho Lee. Unsupervised accuracy estimation of deep visual models using domain-adaptive adversarial perturbation without source samples. In *Proceedings of the IEEE/CVF International Conference on Computer Vision*, pages 16443–16452, 2023.
- [46] Muiyang Li, Xiaobo Xia, Runze Wu, Fengming Huang, Jun Yu, Bo Han, and Tongliang Liu. Towards realistic model selection for semi-supervised learning. In *Forty-first International Conference on Machine Learning*, 2024.
- [47] Yuzhe Lu, Yilong Qin, Runtian Zhai, Andrew Shen, Ketong Chen, Zhenlin Wang, Soheil Kolouri, Simon Stepputtis, Joseph Campbell, and Katia Sycara. Characterizing out-of-distribution error via optimal transport. *Advances in Neural Information Processing Systems*, 36:17602–17622, 2023.
- [48] John P Miller, Rohan Taori, Aditi Raghunathan, Shiori Sagawa, Pang Wei Koh, Vaishaal Shankar, Percy Liang, Yair Carmon, and Ludwig Schmidt. Accuracy on the line: on the strong correlation between out-of-distribution and in-distribution generalization. In *International conference on machine learning*, pages 7721–7735. PMLR, 2021.
- [49] Rajiv Movva, Pang Wei Koh, and Emma Pierson. Using unlabeled data to enhance fairness of medical ai. *Nature Medicine*, 30(4):944–945, 2024.
- [50] Rajiv Movva, Divya Shanmugam, Kaihua Hou, Priya Pathak, John Gutttag, Nikhil Garg, and Emma Pierson. Coarse race data conceals disparities in clinical risk score performance. In *Machine Learning for Healthcare Conference*, pages 443–472. PMLR, 2023.

- [51] Alfredo Nazabal, Pablo Garcia-Moreno, Antonio Artes-Rodriguez, and Zoubin Ghahramani. Human Activity Recognition by Combining a Small Number of Classifiers. *IEEE journal of biomedical and health informatics*, 20(5):1342–1351, September 2016.
- [52] Fabio Parisi, Francesco Strino, Boaz Nadler, and Yuval Kluger. Ranking and combining multiple predictors without labeled data. *Proceedings of the National Academy of Sciences*, 111(4):1253–1258, 2014.
- [53] Vera Pawlowsky-Glahn and Antonella Buccianti. *Compositional data analysis*. Wiley Online Library, 2011.
- [54] F. Pedregosa, G. Varoquaux, A. Gramfort, V. Michel, B. Thirion, O. Grisel, M. Blondel, P. Prettenhofer, R. Weiss, V. Dubourg, J. Vanderplas, A. Passos, D. Cournapeau, M. Brucher, M. Perrot, and E. Duchesnay. Scikit-learn: Machine learning in Python. *Journal of Machine Learning Research*, 12:2825–2830, 2011.
- [55] Emma Pierson, Pang Wei Koh, Tatsunori Hashimoto, Daphne Koller, Jure Leskovec, Nick Eriksson, and Percy Liang. Inferring multidimensional rates of aging from cross-sectional data. In *The 22nd International Conference on Artificial Intelligence and Statistics*, pages 97–107. PMLR, 2019.
- [56] Gregor Pirš and Erik Štrumbelj. Bayesian Combination of Probabilistic Classifiers using Multivariate Normal Mixtures. *Journal of Machine Learning Research*, 20(51):1–18, 2019.
- [57] Emmanouil Platanios, Hoifung Poon, Tom M Mitchell, and Eric J Horvitz. Estimating accuracy from unlabeled data: A probabilistic logic approach. *Advances in neural information processing systems*, 30, 2017.
- [58] Alexander Ratner, Stephen H Bach, Henry Ehrenberg, Jason Fries, Sen Wu, and Christopher Ré. Snorkel: Rapid training data creation with weak supervision. In *Proceedings of the VLDB endowment. International conference on very large data bases*, volume 11, page 269. NIH Public Access, 2017.
- [59] Joel Ratsaby and Santosh S Venkatesh. Learning from a mixture of labeled and unlabeled examples with parametric side information. In *Proceedings of the eighth annual conference on Computational learning theory*, pages 412–417, 1995.
- [60] Philippe Rigollet. Generalization error bounds in semi-supervised classification under the cluster assumption. *Journal of Machine Learning Research*, 8(7), 2007.
- [61] Shiori Sagawa, Pang Wei Koh, Tony Lee, Irena Gao, Sang Michael Xie, Kendrick Shen, Ananya Kumar, Weihua Hu, Michihiro Yasunaga, Henrik Marklund, et al. Extending the wilds benchmark for unsupervised adaptation. *arXiv preprint arXiv:2112.05090*, 2021.
- [62] Kuniaki Saito, Donghyun Kim, Piotr Teterwak, Stan Sclaroff, Trevor Darrell, and Kate Saenko. Tune it the right way: Unsupervised validation of domain adaptation via soft neighborhood density. In *Proceedings of the IEEE/CVF international conference on computer vision*, pages 9184–9193, 2021.
- [63] V Sanh. Distilbert, a distilled version of bert: Smaller, faster, cheaper and lighter. *arXiv preprint arXiv:1910.01108*, 2019.
- [64] Jacob Steinhardt and Percy S Liang. Unsupervised Risk Estimation Using Only Conditional Independence Structure. In *Advances in Neural Information Processing Systems*, volume 29. Curran Associates, Inc., 2016.
- [65] Vincent Stimper, Bernhard Schölkopf, and José Miguel Hernández-Lobato. Resampling base distributions of normalizing flows. In *International Conference on Artificial Intelligence and Statistics*, pages 4915–4936. PMLR, 2022.
- [66] Xiaofei Sun, Xiaoya Li, Jiwei Li, Fei Wu, Shangwei Guo, Tianwei Zhang, and Guoyin Wang. Text classification via large language models. *arXiv preprint arXiv:2305.08377*, 2023.

- [67] Alexandru Tifrea, Gizem Yüce, Amartya Sanyal, and Fanny Yang. Can semi-supervised learning use all the data effectively? a lower bound perspective. In A. Oh, T. Naumann, A. Globerson, K. Saenko, M. Hardt, and S. Levine, editors, *Advances in Neural Information Processing Systems*, volume 36, pages 21960–21982. Curran Associates, Inc., 2023.
- [68] Petter Törnberg. Large language models outperform expert coders and supervised classifiers at annotating political social media messages. *Social Science Computer Review*, page 08944393241286471, 2024.
- [69] Peter Welinder, Max Welling, and Pietro Perona. A Lazy Man’s Approach to Benchmarking: Semisupervised Classifier Evaluation and Recalibration. In *2013 IEEE Conference on Computer Vision and Pattern Recognition*, pages 3262–3269, June 2013. ISSN: 1063-6919.
- [70] Adina Williams, Nikita Nangia, and Samuel Bowman. A broad-coverage challenge corpus for sentence understanding through inference. In *Proceedings of the 2018 Conference of the North American Chapter of the Association for Computational Linguistics: Human Language Technologies, Volume 1 (Long Papers)*, pages 1112–1122, 2018.
- [71] Xixin Wu and Mark Gales. Should ensemble members be calibrated? *arXiv preprint arXiv:2101.05397*, 2021.
- [72] Feng Xie, Jun Zhou, Jin Wee Lee, Mingrui Tan, Siqi Li, Logasan S/O Rajnthern, Marcel Lucas Chee, Bibhas Chakraborty, An-Kwok Ian Wong, Alon Dagan, Marcus Eng Hock Ong, Fei Gao, and Nan Liu. Benchmarking emergency department prediction models with machine learning and public electronic health records. *Scientific Data*, 9:658, October 2022.
- [73] Yuzhe Yang, Haoran Zhang, Dina Katabi, and Marzyeh Ghassemi. Change is hard: A closer look at subpopulation shift. In *International Conference on Machine Learning*, pages 39584–39622. PMLR, 2023.
- [74] Fanghua Ye, Mingming Yang, Jianhui Pang, Longyue Wang, Derek F Wong, Emine Yilmaz, Shuming Shi, and Zhaopeng Tu. Benchmarking llms via uncertainty quantification. *arXiv preprint arXiv:2401.12794*, 2024.
- [75] Xiang Zhang, Junbo Zhao, and Yann LeCun. Character-level convolutional networks for text classification. *Advances in neural information processing systems*, 28, 2015.
- [76] Bingchen Zhao, Xin Wen, and Kai Han. Learning semi-supervised gaussian mixture models for generalized category discovery. In *Proceedings of the IEEE/CVF International Conference on Computer Vision*, pages 16623–16633, 2023.
- [77] Lianmin Zheng, Wei-Lin Chiang, Ying Sheng, Siyuan Zhuang, Zhanghao Wu, Yonghao Zhuang, Zi Lin, Zhuohan Li, Dacheng Li, Eric Xing, et al. Judging llm-as-a-judge with mt-bench and chatbot arena. *Advances in Neural Information Processing Systems*, 36:46595–46623, 2023.
- [78] Caleb Ziems, William Held, Omar Shaikh, Jiaao Chen, Zhehao Zhang, and Diyi Yang. Can large language models transform computational social science? *Computational Linguistics*, 50(1):237–291, 2024.

NeurIPS Paper Checklist

The checklist is designed to encourage best practices for responsible machine learning research, addressing issues of reproducibility, transparency, research ethics, and societal impact. Do not remove the checklist: **The papers not including the checklist will be desk rejected.** The checklist should follow the references and follow the (optional) supplemental material. The checklist does NOT count towards the page limit.

Please read the checklist guidelines carefully for information on how to answer these questions. For each question in the checklist:

- You should answer [Yes], [No], or [NA].
- [NA] means either that the question is Not Applicable for that particular paper or the relevant information is Not Available.
- Please provide a short (1–2 sentence) justification right after your answer (even for NA).

The checklist answers are an integral part of your paper submission. They are visible to the reviewers, area chairs, senior area chairs, and ethics reviewers. You will be asked to also include it (after eventual revisions) with the final version of your paper, and its final version will be published with the paper.

The reviewers of your paper will be asked to use the checklist as one of the factors in their evaluation. While "[Yes]" is generally preferable to "[No]", it is perfectly acceptable to answer "[No]" provided a proper justification is given (e.g., "error bars are not reported because it would be too computationally expensive" or "we were unable to find the license for the dataset we used"). In general, answering "[No]" or "[NA]" is not grounds for rejection. While the questions are phrased in a binary way, we acknowledge that the true answer is often more nuanced, so please just use your best judgment and write a justification to elaborate. All supporting evidence can appear either in the main paper or the supplemental material, provided in appendix. If you answer [Yes] to a question, in the justification please point to the section(s) where related material for the question can be found.

1. Claims

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

Answer: [Yes]

Justification: We acknowledge in our introduction the past work that we build upon (i.e., prior work captures subsets of information that we use) while introducing our method. We also support our claims with empirical experiments and mention the top-level results in the abstract and intro.

Guidelines:

- The answer NA means that the abstract and introduction do not include the claims made in the paper.
- The abstract and/or introduction should clearly state the claims made, including the contributions made in the paper and important assumptions and limitations. A No or NA answer to this question will not be perceived well by the reviewers.
- The claims made should match theoretical and experimental results, and reflect how much the results can be expected to generalize to other settings.
- It is fine to include aspirational goals as motivation as long as it is clear that these goals are not attained by the paper.

2. Limitations

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

Answer: [Yes]

Justification: We state clearly limiting assumptions to our theory and also note when our model doesn't outperform baselines.

Guidelines:

- The answer NA means that the paper has no limitation while the answer No means that the paper has limitations, but those are not discussed in the paper.
- The authors are encouraged to create a separate "Limitations" section in their paper.
- The paper should point out any strong assumptions and how robust the results are to violations of these assumptions (e.g., independence assumptions, noiseless settings, model well-specification, asymptotic approximations only holding locally). The authors should reflect on how these assumptions might be violated in practice and what the implications would be.
- The authors should reflect on the scope of the claims made, e.g., if the approach was only tested on a few datasets or with a few runs. In general, empirical results often depend on implicit assumptions, which should be articulated.
- The authors should reflect on the factors that influence the performance of the approach. For example, a facial recognition algorithm may perform poorly when image resolution is low or images are taken in low lighting. Or a speech-to-text system might not be used reliably to provide closed captions for online lectures because it fails to handle technical jargon.
- The authors should discuss the computational efficiency of the proposed algorithms and how they scale with dataset size.
- If applicable, the authors should discuss possible limitations of their approach to address problems of privacy and fairness.
- While the authors might fear that complete honesty about limitations might be used by reviewers as grounds for rejection, a worse outcome might be that reviewers discover limitations that aren't acknowledged in the paper. The authors should use their best judgment and recognize that individual actions in favor of transparency play an important role in developing norms that preserve the integrity of the community. Reviewers will be specifically instructed to not penalize honesty concerning limitations.

3. Theory assumptions and proofs

Question: For each theoretical result, does the paper provide the full set of assumptions and a complete (and correct) proof?

Answer: [\[Yes\]](#)

Justification: We state that our theory requires assuming a different optimization algorithm (UL+) than the one we use (EM). We also limit our theory to the binary classification case but state this clearly.

Guidelines:

- The answer NA means that the paper does not include theoretical results.
- All the theorems, formulas, and proofs in the paper should be numbered and cross-referenced.
- All assumptions should be clearly stated or referenced in the statement of any theorems.
- The proofs can either appear in the main paper or the supplemental material, but if they appear in the supplemental material, the authors are encouraged to provide a short proof sketch to provide intuition.
- Inversely, any informal proof provided in the core of the paper should be complemented by formal proofs provided in appendix or supplemental material.
- Theorems and Lemmas that the proof relies upon should be properly referenced.

4. Experimental result reproducibility

Question: Does the paper fully disclose all the information needed to reproduce the main experimental results of the paper to the extent that it affects the main claims and/or conclusions of the paper (regardless of whether the code and data are provided or not)?

Answer: [\[Yes\]](#)

Justification: We provide the names and tasks of all datasets used in the paper. We are not releasing code now as per the anonymity policy but are happy to provide it upon request.

Guidelines:

- The answer NA means that the paper does not include experiments.

- If the paper includes experiments, a No answer to this question will not be perceived well by the reviewers: Making the paper reproducible is important, regardless of whether the code and data are provided or not.
- If the contribution is a dataset and/or model, the authors should describe the steps taken to make their results reproducible or verifiable.
- Depending on the contribution, reproducibility can be accomplished in various ways. For example, if the contribution is a novel architecture, describing the architecture fully might suffice, or if the contribution is a specific model and empirical evaluation, it may be necessary to either make it possible for others to replicate the model with the same dataset, or provide access to the model. In general, releasing code and data is often one good way to accomplish this, but reproducibility can also be provided via detailed instructions for how to replicate the results, access to a hosted model (e.g., in the case of a large language model), releasing of a model checkpoint, or other means that are appropriate to the research performed.
- While NeurIPS does not require releasing code, the conference does require all submissions to provide some reasonable avenue for reproducibility, which may depend on the nature of the contribution. For example
 - (a) If the contribution is primarily a new algorithm, the paper should make it clear how to reproduce that algorithm.
 - (b) If the contribution is primarily a new model architecture, the paper should describe the architecture clearly and fully.
 - (c) If the contribution is a new model (e.g., a large language model), then there should either be a way to access this model for reproducing the results or a way to reproduce the model (e.g., with an open-source dataset or instructions for how to construct the dataset).
 - (d) We recognize that reproducibility may be tricky in some cases, in which case authors are welcome to describe the particular way they provide for reproducibility. In the case of closed-source models, it may be that access to the model is limited in some way (e.g., to registered users), but it should be possible for other researchers to have some path to reproducing or verifying the results.

5. Open access to data and code

Question: Does the paper provide open access to the data and code, with sufficient instructions to faithfully reproduce the main experimental results, as described in supplemental material?

Answer: [Yes]

Justification: Our code is available at <https://github.com/divyashan/SSME>. Most of the data we use is open-access and does not require credentials. MIMIC-IV does require credentialed access but we describe which datasets within MIMIC-IV we use. We explain our datasets in detail in the Datasets section of the main text.

Guidelines:

- The answer NA means that paper does not include experiments requiring code.
- Please see the NeurIPS code and data submission guidelines (<https://nips.cc/public/guides/CodeSubmissionPolicy>) for more details.
- While we encourage the release of code and data, we understand that this might not be possible, so “No” is an acceptable answer. Papers cannot be rejected simply for not including code, unless this is central to the contribution (e.g., for a new open-source benchmark).
- The instructions should contain the exact command and environment needed to run to reproduce the results. See the NeurIPS code and data submission guidelines (<https://nips.cc/public/guides/CodeSubmissionPolicy>) for more details.
- The authors should provide instructions on data access and preparation, including how to access the raw data, preprocessed data, intermediate data, and generated data, etc.
- The authors should provide scripts to reproduce all experimental results for the new proposed method and baselines. If only a subset of experiments are reproducible, they should state which ones are omitted from the script and why.

- At submission time, to preserve anonymity, the authors should release anonymized versions (if applicable).
- Providing as much information as possible in supplemental material (appended to the paper) is recommended, but including URLs to data and code is permitted.

6. Experimental setting/details

Question: Does the paper specify all the training and test details (e.g., data splits, hyper-parameters, how they were chosen, type of optimizer, etc.) necessary to understand the results?

Answer: [\[Yes\]](#)

Justification: We provide experimental details in Appendix B, including datasets and implementations of baselines. We report our splits in Section 4.3: Evaluation.

Guidelines:

- The answer NA means that the paper does not include experiments.
- The experimental setting should be presented in the core of the paper to a level of detail that is necessary to appreciate the results and make sense of them.
- The full details can be provided either with the code, in appendix, or as supplemental material.

7. Experiment statistical significance

Question: Does the paper report error bars suitably and correctly defined or other appropriate information about the statistical significance of the experiments?

Answer: [\[Yes\]](#)

Justification: We report 95% CIs using standard errors computed across 50 randomized data splits in the supplement (Table S3-S8).

Guidelines:

- The answer NA means that the paper does not include experiments.
- The authors should answer "Yes" if the results are accompanied by error bars, confidence intervals, or statistical significance tests, at least for the experiments that support the main claims of the paper.
- The factors of variability that the error bars are capturing should be clearly stated (for example, train/test split, initialization, random drawing of some parameter, or overall run with given experimental conditions).
- The method for calculating the error bars should be explained (closed form formula, call to a library function, bootstrap, etc.)
- The assumptions made should be given (e.g., Normally distributed errors).
- It should be clear whether the error bar is the standard deviation or the standard error of the mean.
- It is OK to report 1-sigma error bars, but one should state it. The authors should preferably report a 2-sigma error bar than state that they have a 96% CI, if the hypothesis of Normality of errors is not verified.
- For asymmetric distributions, the authors should be careful not to show in tables or figures symmetric error bars that would yield results that are out of range (e.g. negative error rates).
- If error bars are reported in tables or plots, The authors should explain in the text how they were calculated and reference the corresponding figures or tables in the text.

8. Experiments compute resources

Question: For each experiment, does the paper provide sufficient information on the computer resources (type of compute workers, memory, time of execution) needed to reproduce the experiments?

Answer: [\[Yes\]](#)

Justification: All experiments can be done on a standard laptop without GPU access.

Guidelines:

- The answer NA means that the paper does not include experiments.
- The paper should indicate the type of compute workers CPU or GPU, internal cluster, or cloud provider, including relevant memory and storage.
- The paper should provide the amount of compute required for each of the individual experimental runs as well as estimate the total compute.
- The paper should disclose whether the full research project required more compute than the experiments reported in the paper (e.g., preliminary or failed experiments that didn't make it into the paper).

9. Code of ethics

Question: Does the research conducted in the paper conform, in every respect, with the NeurIPS Code of Ethics <https://neurips.cc/public/EthicsGuidelines>?

Answer: [Yes]

Justification: We have preserved anonymity and checked for compliance with the Code of Ethics.

Guidelines:

- The answer NA means that the authors have not reviewed the NeurIPS Code of Ethics.
- If the authors answer No, they should explain the special circumstances that require a deviation from the Code of Ethics.
- The authors should make sure to preserve anonymity (e.g., if there is a special consideration due to laws or regulations in their jurisdiction).

10. Broader impacts

Question: Does the paper discuss both potential positive societal impacts and negative societal impacts of the work performed?

Answer: [Yes]

Justification: We discuss how this work can be used in various settings, including healthcare, content moderation, and subgroup-specific performance estimation.

Guidelines:

- The answer NA means that there is no societal impact of the work performed.
- If the authors answer NA or No, they should explain why their work has no societal impact or why the paper does not address societal impact.
- Examples of negative societal impacts include potential malicious or unintended uses (e.g., disinformation, generating fake profiles, surveillance), fairness considerations (e.g., deployment of technologies that could make decisions that unfairly impact specific groups), privacy considerations, and security considerations.
- The conference expects that many papers will be foundational research and not tied to particular applications, let alone deployments. However, if there is a direct path to any negative applications, the authors should point it out. For example, it is legitimate to point out that an improvement in the quality of generative models could be used to generate deepfakes for disinformation. On the other hand, it is not needed to point out that a generic algorithm for optimizing neural networks could enable people to train models that generate Deepfakes faster.
- The authors should consider possible harms that could arise when the technology is being used as intended and functioning correctly, harms that could arise when the technology is being used as intended but gives incorrect results, and harms following from (intentional or unintentional) misuse of the technology.
- If there are negative societal impacts, the authors could also discuss possible mitigation strategies (e.g., gated release of models, providing defenses in addition to attacks, mechanisms for monitoring misuse, mechanisms to monitor how a system learns from feedback over time, improving the efficiency and accessibility of ML).

11. Safeguards

Question: Does the paper describe safeguards that have been put in place for responsible release of data or models that have a high risk for misuse (e.g., pretrained language models, image generators, or scraped datasets)?

Answer: [NA]

Justification: We do not think this work could be directly used for misuse.

Guidelines:

- The answer NA means that the paper poses no such risks.
- Released models that have a high risk for misuse or dual-use should be released with necessary safeguards to allow for controlled use of the model, for example by requiring that users adhere to usage guidelines or restrictions to access the model or implementing safety filters.
- Datasets that have been scraped from the Internet could pose safety risks. The authors should describe how they avoided releasing unsafe images.
- We recognize that providing effective safeguards is challenging, and many papers do not require this, but we encourage authors to take this into account and make a best faith effort.

12. Licenses for existing assets

Question: Are the creators or original owners of assets (e.g., code, data, models), used in the paper, properly credited and are the license and terms of use explicitly mentioned and properly respected?

Answer: [Yes]

Justification: We cite previous code and data with URLs and in-text paper citations.

Guidelines:

- The answer NA means that the paper does not use existing assets.
- The authors should cite the original paper that produced the code package or dataset.
- The authors should state which version of the asset is used and, if possible, include a URL.
- The name of the license (e.g., CC-BY 4.0) should be included for each asset.
- For scraped data from a particular source (e.g., website), the copyright and terms of service of that source should be provided.
- If assets are released, the license, copyright information, and terms of use in the package should be provided. For popular datasets, paperswithcode.com/datasets has curated licenses for some datasets. Their licensing guide can help determine the license of a dataset.
- For existing datasets that are re-packaged, both the original license and the license of the derived asset (if it has changed) should be provided.
- If this information is not available online, the authors are encouraged to reach out to the asset's creators.

13. New assets

Question: Are new assets introduced in the paper well documented and is the documentation provided alongside the assets?

Answer: [NA]

Justification: We do not release new assets other than code, which we discussed in a previous response.

Guidelines:

- The answer NA means that the paper does not release new assets.
- Researchers should communicate the details of the dataset/code/model as part of their submissions via structured templates. This includes details about training, license, limitations, etc.
- The paper should discuss whether and how consent was obtained from people whose asset is used.
- At submission time, remember to anonymize your assets (if applicable). You can either create an anonymized URL or include an anonymized zip file.

14. Crowdsourcing and research with human subjects

Question: For crowdsourcing experiments and research with human subjects, does the paper include the full text of instructions given to participants and screenshots, if applicable, as well as details about compensation (if any)?

Answer: [NA]

Justification: We did not crowdsource any data.

Guidelines:

- The answer NA means that the paper does not involve crowdsourcing nor research with human subjects.
- Including this information in the supplemental material is fine, but if the main contribution of the paper involves human subjects, then as much detail as possible should be included in the main paper.
- According to the NeurIPS Code of Ethics, workers involved in data collection, curation, or other labor should be paid at least the minimum wage in the country of the data collector.

15. **Institutional review board (IRB) approvals or equivalent for research with human subjects**

Question: Does the paper describe potential risks incurred by study participants, whether such risks were disclosed to the subjects, and whether Institutional Review Board (IRB) approvals (or an equivalent approval/review based on the requirements of your country or institution) were obtained?

Answer: [NA]

Justification: This research does not directly involve human subjects. We received proper approval for datasets involving human subjects.

Guidelines:

- The answer NA means that the paper does not involve crowdsourcing nor research with human subjects.
- Depending on the country in which research is conducted, IRB approval (or equivalent) may be required for any human subjects research. If you obtained IRB approval, you should clearly state this in the paper.
- We recognize that the procedures for this may vary significantly between institutions and locations, and we expect authors to adhere to the NeurIPS Code of Ethics and the guidelines for their institution.
- For initial submissions, do not include any information that would break anonymity (if applicable), such as the institution conducting the review.

16. **Declaration of LLM usage**

Question: Does the paper describe the usage of LLMs if it is an important, original, or non-standard component of the core methods in this research? Note that if the LLM is used only for writing, editing, or formatting purposes and does not impact the core methodology, scientific rigor, or originality of the research, declaration is not required.

Answer: [NA]

Justification: We used LLMs to make edits to figures, tables, writing, and code. However, we did not directly use LLMs to build the core methodology presented in the paper.

Guidelines:

- The answer NA means that the core method development in this research does not involve LLMs as any important, original, or non-standard components.
- Please refer to our LLM policy (<https://neurips.cc/Conferences/2025/LLM>) for what should or should not be described.

Appendix

A Related work

We detail related work in unsupervised performance estimation here. Works below assume access to *only* unlabeled data; in contrast, SSME learns from both labeled and unlabeled data.

Unsupervised performance estimation involves estimating the performance of a model given only unlabeled data. Methods designed to address this problem often focus on out-of-distribution samples, where labeled data is scarce and model performance is known to degrade. Several works have illustrated strong empirical relationships between out-of-distribution generalization and thresholded classifier confidence [28], dataset characteristics [21, 30], in-distribution classifier accuracy [48], and classifier agreement [52, 57, 5].

Several works have formalized when unsupervised model evaluation is possible [23, 13, 28, 47, 73, 20, 62], and propose assumptions under which estimates of performance are recoverable. [23] and [6] assume knowledge of $p(y)$ in the unlabeled sample. [64] assume conditionally-independent subsets of the observed features, inspired by conditional-independence assumptions made in works such as [18]. [30] assume classifier calibration on unlabeled samples. [13] assume a sparse covariate shift model, in which a subset of the features' class-conditional distribution remains constant. [47] illustrate misestimation of $p(y)$ in the unlabeled example, and assume that $p(y)$ out-of-distribution is close to $p(y)$ in-distribution. As [28] highlight, assumptions are necessary to make any claim about the nature of unsupervised model evaluation, and the above methods are a representative sample of assumptions made. Finally, there has been a surge of interest in unsupervised performance estimation in the context of large language models [77, 34]. A standard approach here is to use a large language model to adjudicate the quality of text generated by other language models. Methods in this literature are often specific to large language models, while SSME is not.

Our work is also similar, in spirit, to methods that learn to debias classifier predictions on a small set of labeled data and then apply that debiasing procedure to classifier predictions on unlabeled examples. Prediction-powered inference [3] and double machine learning [14] both learn a debiasing procedure to ensure that unlabeled metric estimates (e.g., accuracy) are statistically unbiased. One of the baselines we compare to, AutoEval [11], is built atop prediction-powered inference.

B Experimental details

We provide an extensible implementation of SSME at <https://github.com/divyashan/SSME>, along with support for applying SSME to your own setting. Below, we provide additional detail on the experiments reported in the main text.

B.1 Real datasets and classifier sets

We provide additional detail for the five datasets we use in our work, including ground truth $p(y)$ for each dataset and ground truth metrics for each classifier in the associated classifier set in Table S1 and Table S2. As discussed, each dataset is split into a training split (provided to each classifier as training data), an estimation split (provided to each performance estimation method), and an evaluation split (used to compute ground truth metrics for each classifier). We determine training splits based on prior work. We then split the remaining data in half (randomly, for each run) to produce the estimation and evaluation splits. We then subsample the estimation split to have n_l labeled examples and n_u unlabeled examples. We ensure that the labeled data always includes at least one example from each class. Thus, the estimation split contains $n_l + n_u$ examples in each experiment, and the evaluation split for each task is fixed across runs (exact sample sizes reported below). No performance estimation method sees data from the evaluation split, which is used to evaluate the performance estimates.

1. **MIMIC-IV**: We use three binary classification tasks from MIMIC-IV [38], a large dataset of electronic health records describing 418K patient visits to an emergency department. We focus on three tasks: **hospitalization** (predicting hospital admission based on features available during triage, $p(y = 1) = 0.45$), **critical outcomes** (predicting inpatient mortality or a transfer to the ICU within 12 hours, $p(y = 1) = 0.06$), and **emergency department revisits** (predicting a patient's return to the emergency department within 3 days, $p(y =$

- 1) = 0.03). We split and preprocess data according to prior work [72, 50]. No patient appears in more than one split. For each task, the evaluation split contains 70,439 examples. The classifiers in the associated set differ by function class (logistic regression, decision tree, and multi-layer perceptron) and random seed (0, 1, 2).
2. **Toxicity detection:** The task is to predict presence of toxicity given an online comment, using data from CivilComments [9, 42] where $p(y = 1) = 0.11$. The evaluation split contains 66,891 examples. The classifiers in the associated set differ by training loss (ERM, IRM, and CORAL) and random seed (0, 1, 2).
 3. **Biochemical property prediction** The task is to predict presence of a biochemical property based on a molecular graph, using data from the Open Graph Benchmark [33]. We focus on the task of predicting whether a molecule inhibits SARS-CoV virus maturation, where $p(y = 1) = 0.09$. We filter out examples for which *no* label is observed (i.e. the molecule was not screened at all) because it is impossible to evaluate our performance estimates on those examples. Doing so reduces data held-out from training from 43,793 to 28,325 examples. The evaluation split then contains half, or 14,163, of those examples. The classifiers in the associated set differ by training loss (ERM, IRM, and CORAL) and random seed (0, 1, 2).
 4. **News classification** The task is to predict one of four news types based on the title and description of an article [75]. The dataset contains 7,600 examples, with 2,550 examples reserved for the evaluation split. The classes are balanced. Classifiers differ by the base LLM used to perform news classification. The first LLM is Llama-3.2-3B-Instruct, and we obtain probabilities over all classes through zero-shot prompting (i.e. providing one example at a time, accompanied by options) using code provided by [74]. The three remaining LLMs are closed-source models provided by OpenAI: text-embedding-3-small, text-embedding-3-large, and text-embedding-ada-002. We train a classifier atop these embeddings by training a multiclass logistic regression on 2,500 embeddings of labeled examples.
 5. **Sentence classification** The task is to predict one of three textual entailments from a sentence [70]. The classes are balanced and the evaluation split contains 61,856 examples. Classifiers differ by training loss (ReWeight, ReSample, IRM, and SqrtReWeight) according to [73].

SSME, in contrast to prior work, makes no assumption about the correlation between classifiers because any assumption is unlikely to hold in practice. The average correlation between classifiers in our sets for each binary task is 0.53, 0.85, 0.93, 0.81, 0.77 (for ED revisit, critical outcome, hospitalization, toxicity, and SARS-COV inhibition prediction respectively). This range of values reflects natural correlation between classifiers in practice, since each of our models is either an off-the-shelf classifier or trained using publicly available code.

B.2 Baselines

For baselines that require discrete predictions (i.e. Dawid-Skene and AutoEval), we discretize classifier scores by assigning a class according to the maximum classifier score across classes. We expand on our implementation of each baseline below.

- *Labeled:* When estimating performance over the whole dataset, we compare the classifier scores to the ground truth labels within the labeled sample. However, when estimating subgroup-specific performance, it is often the case that there are no labeled examples for a given subgroup. In these instances, *Labeled* reverts to estimating subgroup-specific performance as performance over all labeled examples.
- *Pseudo-Labeling (PL):* We train a logistic regression with the default parameters associated with the scikit-learn implementation [54]. Experiments with alternative function classes (e.g. a KNN) revealed no significant differences in performance.
- *Bayesian-Calibration (BC):* Bayesian-Calibration operates on each classifier individually. We make use of the implementation made available by [37]. Extending the proposed approach to multi-class tasks is not straightforward, so we compare to *Bayesian-Calibration* only on binary tasks. We compare to *Bayesian-Calibration* on binary tasks, as it does not extend naturally to multiclass settings.
- *SPE:* SPE [69] is a semi-supervised single classifier evaluation method that relies on parametric assumptions about the distribution of classifier scores. They find that the truncated

Dataset	Classifier	Acc	ECE	AUC	AUPRC
Hospital Admission	DT-RandomForest-seed1	74.2	1.5	81.5	76.0
	MLP-ERM-seed2	74.4	1.4	81.7	76.7
	MLP-ERM-seed1	74.4	1.9	81.9	77.0
	MLP-ERM-seed0	74.5	2.4	82.0	77.0
	LR-LBFGS-seed2	73.3	4.0	80.7	75.5
	LR-LBFGS-seed1	73.3	4.0	80.7	75.5
	LR-LBFGS-seed0	73.4	2.9	81.0	75.7
	DT-RandomForest-seed2	74.3	1.6	81.5	76.1
Critical Outcome	DT-RandomForest-seed0	74.1	1.5	81.5	76.1
	MLP-ERM-seed2	93.9	0.9	87.9	38.6
	MLP-ERM-seed1	93.9	0.8	88.1	39.0
	LR-LBFGS-seed2	93.6	1.2	87.6	34.2
	MLP-ERM-seed0	93.9	0.5	87.5	37.8
	LR-LBFGS-seed0	93.6	1.2	87.6	34.1
	DT-RandomForest-seed2	94.0	0.3	87.2	38.2
	DT-RandomForest-seed1	94.0	0.4	87.4	38.3
ED Revisit	DT-RandomForest-seed0	94.0	0.4	87.4	38.3
	LR-LBFGS-seed1	93.6	1.2	87.6	34.2
	DT-RandomForest-seed0	97.7	1.8	54.9	2.7
	DT-RandomForest-seed1	97.7	1.7	55.3	2.7
	DT-RandomForest-seed2	97.7	1.8	54.9	2.7
	LR-LBFGS-seed0	97.7	0.4	59.3	3.0
	LR-LBFGS-seed2	97.7	0.4	59.1	3.0
	MLP-ERM-seed0	97.7	0.3	59.8	3.1
Toxicity Detection	MLP-ERM-seed1	97.7	0.3	59.8	3.1
	MLP-ERM-seed2	97.7	0.5	57.9	3.0
	LR-LBFGS-seed1	97.7	0.4	59.1	3.0
	distilbert-CORAL-seed0	88.3	6.0	86.2	40.0
	distilbert-IRM-seed2	88.7	10.2	91.9	65.5
	distilbert-IRM-seed1	89.0	9.8	91.0	66.5
	distilbert-IRM-seed0	88.1	10.6	91.6	65.9
	distilbert-ERM-seed2	92.1	4.9	94.1	73.3
Molecule Property 60	distilbert-ERM-seed1	92.2	6.2	93.8	72.3
	distilbert-ERM-seed0	92.2	6.1	93.8	72.2
	gin-virtual-CORAL-seed1	92.8	5.2	90.1	61.9
	gin-virtual-CORAL-seed2	92.8	5.2	90.1	61.9
	gin-virtual-ERM-seed0	94.6	1.2	94.5	73.5
	gin-virtual-ERM-seed1	92.4	5.6	90.7	61.1
	gin-virtual-ERM-seed2	92.8	5.2	90.1	61.9
	gin-virtual-IRM-seed0	93.2	1.8	90.2	58.4
	gin-virtual-IRM-seed1	91.1	5.2	83.8	43.8
	gin-virtual-IRM-seed2	91.1	5.7	82.8	44.7

Table S1: **Ground truth classifier metrics on binary tasks.** We report ground truth performance for classifiers in the sets associated with each binary task. Each classifier name begins with the architecture (e.g. DT represents DecisionTree), the loss or training procedure (e.g. ERM or IRM), and then the seed. Note that the equivalent accuracies on ED Revisit are a byproduct of both the low class prevalence and the poor classifiers.

dataset	model	Acc	ECE
AG News	llama-3.2-3B-Instruct	85.6	8.6
	text-embedding-3-large	90.1	8.8
	text-embedding-3-small	89.8	9.1
	text-embedding-ada-002	89.0	9.3
MultiNLI	distilbert-IRM	64.8	6.1
	distilbert-ReSample	81.4	8.2
	distilbert-ReWeight	80.9	7.4
	distilbert-SqrtReWeight	81.4	9.2

Table S2: **Ground truth classifier metrics on multiclass tasks.** We report ground truth performance for classifiers in the sets associated with each multiclass task. Each of the LLMs fine-tuned for AG News are sentence transformers, while the MultiNLI classifiers all use DistilBERT [63] as the base architecture.

Normal distribution demonstrates reasonable fit across datasets; accordingly, we implement SPE as a mixture of truncated Normal distributions fit to each classifier's predictions individually.

- *Dawid-Skene*: We implement Dawid-Skene with a tolerance of $1e-5$ and a maximum number of EM iterations of 100 (the default parameters), using the following public implementation: https://github.com/dallascard/dawid_skene. Dawid-Skene accepts discrete predictions, so we discretize classifier predictions using thresholding the predicted class probability at $\frac{1}{K}$.
- *Majority-Vote*: We implement Majority-Vote as the accuracy-weighted average of discrete predictions made by each classifier. We discretize predictions by thresholding predicted probabilities at $\frac{1}{K}$. We weight each classifier in proportion to its accuracy on the available labeled data.
- *Active-Testing*: We implement Active-Testing, where the method selects a fixed number of examples to label out of a pool of unlabeled examples, according to the approach proposed by [43]. We select examples according to the acquisition strategy for estimating accuracy, a metric for which a public implementation is available, and limit our comparison to this metric.
- *AutoEval*: We implement AutoEval using an implementation made available by the authors [11]. The implementation, to the best of our knowledge, only supports accuracy estimation across a set of classifiers, so we limit our comparison to this metric. We compare to *AutoEval* on accuracy estimation, as additional metrics are not supported by the public implementation.

B.3 Computing effective sample size

In order to compute effective sample size, we produce 50 samples of labeled data for each increment of 5 between 10 labeled examples and 1000. We then compute the mean absolute metric estimation error of using labeled data alone, across all runs. The effective sample size of a given semi-supervised evaluation method is thus the amount of labeled data which achieves the most similar mean absolute metric estimation error.

C Proof of Theorem 1

We derive a high-probability error bound on performance estimates based on prior results in semi-supervised mixture models [67]. The proof consists of two steps: we first bound the error in estimation of component separation. We then use the relationship between component separation and classifier performance to bound the error in estimating classifier performance.

Model of y and s . We consider a stylized binary classification setting drawn from previous work [67] where classifier scores s are drawn from a balanced mixture of two Gaussians. For data in the positive class, classifier scores are drawn from a multivariate Gaussian. The Gaussian assumption holds when the distribution of classifier logits follows a normal distribution. $\mathcal{N}(\mathbf{c}, I)$, where $\mathbf{c} \in \mathbb{R}^d$. For data in the negative class, classifier scores are drawn from a multivariate Gaussian $\mathcal{N}(0, I)$. Let n_u refer to the number of unlabeled examples, n_ℓ the number of labeled examples, and d the number of classifiers. Additional classifiers increase the dimensionality of the multivariate Gaussian.

Estimator We reason about SSME's performance using a simplified semi-supervised learning algorithm. The estimator, UL+, first uses the unlabeled data to identify decision boundaries, and then uses the labeled data to assign decision boundaries to classes. As the authors note, this is not the most efficient use of labeled data. We expect that using the labeled data in the expectation-maximization procedure – as SSME does – to weakly outperform UL+ because it uses labeled data when learning the decision boundaries. For additional detail on the estimator, please refer to Section 2.3 of [67].

Theorem 1 Let $\widehat{AUC}_k$, $\widehat{ACC}_k$ be estimators for AUC_k , ACC_k , estimated using UL+, and $\mathbf{c}_k$ be the L2 distance between components along dimension k . Assume $n_u \gtrsim \max \left\{ d, \frac{d}{\mathbf{c}^4}, \frac{\log(n_u)}{\min\{\mathbf{c}^2, \mathbf{c}^4\}}, \frac{d \log(d n_u)}{\mathbf{c}^6} \right\}$ and $d \geq 2$. With probability $1 - p$, errors in the estimated AUC and accuracy of classifier k differ by at most:

$$|AUC_k - \widehat{AUC}_k| \leq \Phi\left(\frac{\mathbf{c}_k}{\sqrt{2}}\right) - \Phi\left(\frac{\mathbf{c}_k - \epsilon_{\mathbf{c}}}{\sqrt{2}}\right) \quad (5)$$

$$|ACC_k - \widehat{ACC}_k| \leq \Phi\left(\frac{\mathbf{c}_k}{2}\right) - \Phi\left(\frac{\mathbf{c}_k - \epsilon_{\mathbf{c}}}{2}\right) \quad (6)$$

where $\epsilon_{\mathbf{c}} \lesssim \frac{1}{p} \left(\sqrt{\frac{d}{\|\mathbf{c}\|^2 n_u}} + \|\mathbf{c}\| e^{-\frac{1}{2} n_l \|\mathbf{c}\|^2 \left(1 - \frac{C_0}{\|\mathbf{c}\|^2} \sqrt{\frac{d \log(n_u)}{\|\mathbf{c}\|^2 n_u}}\right)^2} \right)$ and C_0 is a universal constant.

1. Bound error in separation estimation as a function of n_l , n_u , d , and separation $\mathbf{c}$. Prior work [67] has established bounds on the error in mean estimation ϵ_{μ} in the context of a semi-supervised learning algorithm which first uses the unlabeled data to generate decision boundaries, and uses the labeled data to assign labels to regions. The authors prove mean estimation error can be bounded by:

$$\mathbb{E}[\epsilon_{\mu}] \lesssim \sqrt{\frac{d}{\|\mathbf{c}\|^2 n_u}} + \|\mathbf{c}\| e^{-\frac{1}{2} n_l \|\mathbf{c}\|^2 \left(1 - \frac{C_0}{\|\mathbf{c}\|^2} \sqrt{\frac{d \log(n_u)}{\|\mathbf{c}\|^2 n_u}}\right)^2}.$$

where C_0 is some universal constant and not equivalent to $\|\mathbf{c}\|$. We can convert this expectation bound into a high-probability bound using Markov's inequality:

$$\mathbb{P}\left(\epsilon_{\mu} \gtrsim \frac{1}{p} \left(\sqrt{\frac{d}{\|\mathbf{c}\|^2 n_u}} + \|\mathbf{c}\| e^{-\frac{1}{2} n_l \|\mathbf{c}\|^2 \left(1 - \frac{C_0}{\|\mathbf{c}\|^2} \sqrt{\frac{d \log(n_u)}{\|\mathbf{c}\|^2 n_u}}\right)^2} \right)\right) \leq p.$$

Because we pin $\mu_0 = 0$, error in mean estimation is equal to error in separation estimation in this setting, i.e. $\epsilon_{\mu} = \epsilon_{\mathbf{c}}$. So we can state that, with probability $1 - p$, the mean estimation error obeys the following inequality:

$$\epsilon_{\mathbf{c}} \leq \frac{1}{p} \left(\sqrt{\frac{d}{\|\mathbf{c}\|^2 n_u}} + \|\mathbf{c}\| e^{-\frac{1}{2} n_l \|\mathbf{c}\|^2 \left(1 - \frac{C_0}{\|\mathbf{c}\|^2} \sqrt{\frac{d \log(n_u)}{\|\mathbf{c}\|^2 n_u}}\right)^2} \right)$$

2. Bound error in performance estimation. The AUC of the optimal linear classifier (separating classifier predictions for the negative class from classifier predictions in the positive class) is a function of the Mahalanobis distance $\mathbf{c}$, equivalent to the L2 distance in this setting, as prior work has shown [55]:

$$AUC = \Phi\left(\|\mathbf{c}\|/\sqrt{2}\right),$$

where Φ is the cumulative distribution function of the standard normal distribution. Similarly, the accuracy of the optimal linear classifier is:

$$ACC = \Phi(\|\mathbf{c}\|/2)$$

Above, we derived a bound on the error of separation estimation, $\epsilon_{\mathbf{c}}$. Now, we map the error in separation estimation to errors in performance estimation (AUC and accuracy). We can state that the following inequality holds:

$$Pr(\|\mathbf{c}\| - \epsilon_{\mathbf{c}} \leq \|\hat{\mathbf{c}}\| \leq \|\mathbf{c}\| + \epsilon_{\mathbf{c}}) \geq 1 - p$$

Thus:

$$\Phi\left(\frac{\|\mathbf{c}\| - \epsilon_{\mathbf{c}}}{\sqrt{2}}\right) \leq \Phi\left(\frac{\|\hat{\mathbf{c}}\|}{\sqrt{2}}\right) \leq \Phi\left(\frac{\|\mathbf{c}\| + \epsilon_{\mathbf{c}}}{\sqrt{2}}\right) \quad (7)$$

$$\Phi\left(\frac{\|\mathbf{c}\| - \epsilon_{\mathbf{c}}}{\sqrt{2}}\right) \leq \widehat{AUC} \leq \Phi\left(\frac{\|\mathbf{c}\| + \epsilon_{\mathbf{c}}}{\sqrt{2}}\right) \quad (8)$$

$$\Phi\left(\frac{\|\mathbf{c}\| - \epsilon_{\mathbf{c}}}{\sqrt{2}}\right) - \Phi\left(\frac{\|\mathbf{c}\|}{\sqrt{2}}\right) \leq \widehat{AUC} - AUC \leq \Phi\left(\frac{\|\mathbf{c}\| + \epsilon_{\mathbf{c}}}{\sqrt{2}}\right) - \Phi\left(\frac{\|\mathbf{c}\|}{\sqrt{2}}\right) \quad (9)$$

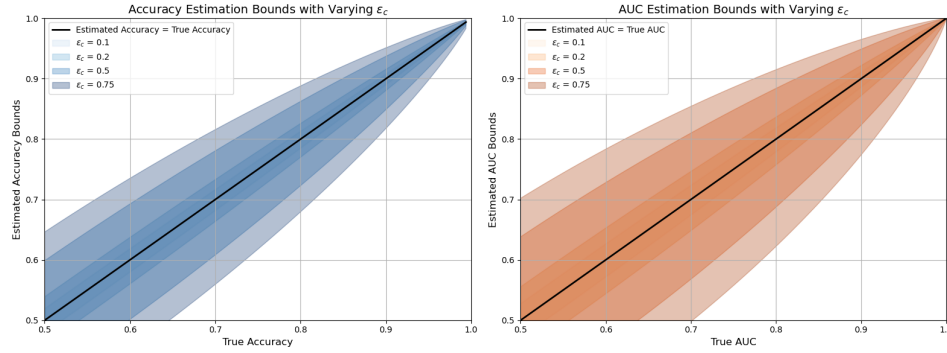


Figure S1: **Estimation error based on original classifier set performance.** We plot estimated classifier performance as a function of original classifier performance for various values of ϵ_c , for accuracy (left) and AUC (right). The less accurate the classifier set, the larger the error bands.

Given that we assume the classifiers are better than random (i.e. $\|\mathbf{c}\| > 0$) the term on the far left of the inequality is larger in magnitude than the term on the far right, so we can simplify as:

$$|\widehat{AUC} - AUC| \leq \max\left(\Phi\left(\frac{\|\mathbf{c}\| + \epsilon_c}{\sqrt{2}}\right) - \Phi\left(\frac{\|\mathbf{c}\|}{\sqrt{2}}\right), \Phi\left(\frac{\|\mathbf{c}\| - \epsilon_c}{\sqrt{2}}\right) - \Phi\left(\frac{\|\mathbf{c}\|}{\sqrt{2}}\right)\right) \quad (10)$$

$$|\widehat{AUC} - AUC| \leq \left|\Phi\left(\frac{\|\mathbf{c}\| - \epsilon_c}{\sqrt{2}}\right) - \Phi\left(\frac{\|\mathbf{c}\|}{\sqrt{2}}\right)\right| \quad (11)$$

Finally, error in estimated separation is necessarily larger than the error in any one dimension, allowing us to state the inequality for each dimension of the mixture. We can also follow the same logic above to derive a bound on error in estimated accuracy. We can state:

$$|\widehat{AUC}_k - AUC_k| \leq \left|\Phi\left(\frac{\mathbf{c}_k}{\sqrt{2}}\right) - \Phi\left(\frac{\mathbf{c}_k - \epsilon_c}{\sqrt{2}}\right)\right| \quad (12)$$

$$|\widehat{ACC}_k - ACC_k| \leq \left|\Phi\left(\frac{\mathbf{c}_k}{2}\right) - \Phi\left(\frac{\mathbf{c}_k - \epsilon_c}{2}\right)\right| \quad (13)$$

where the following holds with probability $1 - p$:

$$\epsilon_c \lesssim \frac{1}{p} \left(\sqrt{\frac{d}{\|\mathbf{c}\|^2 n_u}} + \|\mathbf{c}\| e^{-\frac{1}{2} n_t \|\mathbf{c}\|^2} \left(1 - \frac{C_0}{\|\mathbf{c}\|^2} \sqrt{\frac{d \log(n_u)}{\|\mathbf{c}\|^2 n_u}}\right)^2 \right)$$

We plot bounds in estimated classifier performance as a function of ϵ_c in Fig. S1.

C.1 Impact of additional classifiers

Increasing the number of classifiers impacts the bound in two ways. First, an additional classifier increases the dimensionality d of the mixture model, thereby creating a looser bound. Second, an additional classifier increases the separation between components $\|\mathbf{c}\|$, because each classifier is assumed to be independent from one another. If the marginal increase in separation outweighs the marginal increase to dimensionality, the bound on ϵ_c tightens. Specifically, let's say that the separation of components for the new classifier (i.e. $\mathbf{c}_{k+1}$) is equal to δ . Separation $\|\mathbf{c}\|$ increases to $\sqrt{\|\mathbf{c}\|^2 + \delta^2}$. Dimensionality increases by 1, i.e. $d + 1$. When $\sqrt{\|\mathbf{c}\|^2 + \delta^2}$ exceeds $\sqrt{d + 1}$, the first term in the expression decreases. Specifically:

The norm of the augmented vector $\mathbf{c}' = [\mathbf{c}; \delta]$ exceeds $\sqrt{d + 1}$ if and only if

$$\delta > \sqrt{d + 1 - \|\mathbf{c}\|^2}.$$

If $\|\mathbf{c}\| > \sqrt{d+1}$, then any $\delta > 0$ will result in $\|\mathbf{c}'\| > \sqrt{d+1}$. Otherwise, δ must be large enough to compensate for the square root of the difference between the new dimensionality ($d+1$) and the squared norm ($\|\mathbf{c}\|^2$). At an extreme, if the new classifier is perfectly correlated with another, it increases dimensionality at no benefit to separation between components, resulting in a looser bound.

D Supplementary results

D.1 Results on synthetic data

We corroborate theoretical findings from Section 3.2 in synthetic experiments, including settings where the assumptions do not hold. We draw classifier scores for positive examples from distributions centered on a vector $\mathbf{c}$, where entries of $\mathbf{c}$ are drawn from $N(c, .2)$, enforcing a minimum entry of 0.01 (to ensure that each classifier exhibits performance better than random). We consider $n_u \in 50, 100, 250, 500, 1000, 2000$, $d \in 2, 4, 6, 8, 10$, and $\|\mathbf{c}\| \in 0.75, 1.0, 1.25, 1.5$, and sample 50 datasets for each setting. We provide 20 labeled examples to SSME across all synthetic experiments.

The three theoretical findings we make (using a simplified semi-supervised learning algorithm and a Gaussian assumption) hold in our empirical setting. Our synthetic setting differs from our theoretical setting in two key respects: we use SSME to infer performance and we simulate violations of the Gaussian assumption. Our theoretical findings hold in this more realistic setting; Figure S2 plots results.

D.2 Results reporting mean absolute error

In the main text, we evaluate our method and all baselines using 20 labeled examples and 1000 unlabeled examples and report *rescaled* mean absolute error across metrics and tasks. Here, we supplement those results by reporting mean absolute error across each task and metric and expanding n_l to include 50 and 100. The number of unlabeled examples remains the same (1000) to isolate the effect of additional labeled data.

Tables S3, S4, S5, and S6 report results on each binary task for accuracy, ECE, AUC, and AUPRC, respectively. Three high-level findings emerge. First, SSME-KDE achieves the lowest mean absolute error (averaging across tasks and amounts of labeled data). Second, SSME-KDE consistently outperforms the ablated version of SSME, fit to a single model at a time (SSME-KDE-M). And finally, SSME-KDE is able to produce performance estimates that are quite close, in absolute terms, to ground truth. For example, when given 20 labeled examples and 1000 unlabeled examples, SSME-KDE estimates accuracy within at most 2.5 percentage points of ground truth accuracy (across tasks).

Tables S11 and S12 report our results on the multiclass tasks, for accuracy and ECE respectively. Note that we exclude Bayesian-Calibration from multiclass comparisons because the method does not natively support multiclass recalibration. We also omit AutoEval from Table S12 because the implementation of expected calibration error within the framework is not straightforward.

D.3 Results reporting absolute performance estimates

Results thus far have reported aggregate errors in performance estimates across classifiers in the set. Here, we include results on a per-classifier basis in the context of toxicity detection, the task for which we have the largest variability in classifier quality (Tables S7, S8, S9, S10). The tables illustrate how SSME's performance manifests on a per-classifier basis, often producing more accurate estimates than the baselines on the classifiers with lowest performance. The tables also make evident that SSME's improvement in performance estimation can be attributed to a significant reduction in the variance of performance estimates across different data splits.

D.4 Results reporting robustness to kernel choice

We find that SSME's performance estimates are stable across three kernel choices: a Gaussian kernel, an Epachenikov kernel, and an exponential kernel. Table S13 reports our results in the context of toxicity detection and accuracy, but results generalize across tasks and metrics.

Dataset	n_ℓ	n_u	Labeled	Majority-Vote	PL	Dawid-Skene	SPE	BC	AutoEval	Active-Testing	SSME-M	SSME (Ours)
Critical Outcome	20	1000	5.19 ± 1.07	4.01 ± 0.13	4.12 ± 1.07	4.36 ± 0.09	12.73 ± 5.64	2.80 ± 0.62	4.78 ± 0.93	5.17 ± 0.32	<u>1.70 ± 0.27</u>	0.67 ± 0.13
	50	1000	2.90 ± 0.59	4.21 ± 0.12	3.06 ± 0.64	4.07 ± 0.11	16.79 ± 9.66	2.07 ± 0.36	3.01 ± 0.65	5.61 ± 0.40	<u>1.65 ± 0.25</u>	0.78 ± 0.13
	100	1000	2.09 ± 0.41	4.10 ± 0.14	1.58 ± 0.30	3.87 ± 0.11	8.61 ± 8.84	<u>1.18 ± 0.21</u>	2.00 ± 0.32	5.48 ± 0.35	1.30 ± 0.20	0.77 ± 0.13
ED Revisit	20	1000	5.11 ± 0.98	2.15 ± 0.02	5.13 ± 0.89	4.02 ± 0.78	14.70 ± 10.59	4.36 ± 0.77	4.70 ± 0.92	2.83 ± 0.20	<u>1.64 ± 0.34</u>	0.45 ± 0.10
	50	1000	2.02 ± 0.58	2.10 ± 0.03	2.73 ± 0.62	2.74 ± 0.61	17.96 ± 7.41	2.47 ± 0.57	1.95 ± 0.57	3.03 ± 0.26	<u>1.46 ± 0.27</u>	0.53 ± 0.11
	100	1000	1.43 ± 0.32	2.00 ± 0.05	1.54 ± 0.34	1.51 ± 0.33	11.69 ± 5.13	1.43 ± 0.31	1.42 ± 0.29	2.64 ± 0.16	<u>1.18 ± 0.25</u>	0.57 ± 0.11
Hospital Admission	20	1000	7.32 ± 1.25	16.32 ± 0.66	6.86 ± 1.19	19.55 ± 0.15	14.27 ± 1.76	<u>2.48 ± 0.44</u>	7.19 ± 1.03	9.33 ± 0.84	3.29 ± 0.47	1.88 ± 0.29
	50	1000	5.40 ± 0.83	16.37 ± 0.62	3.99 ± 0.82	18.78 ± 0.16	15.68 ± 0.69	<u>2.14 ± 0.36</u>	5.23 ± 0.68	9.25 ± 0.64	3.17 ± 0.51	1.95 ± 0.27
	100	1000	3.64 ± 0.55	15.34 ± 0.66	3.01 ± 0.53	17.81 ± 0.18	14.32 ± 0.95	<u>2.42 ± 0.33</u>	4.01 ± 0.55	9.24 ± 0.80	3.06 ± 0.45	1.51 ± 0.23
SARS-CoV Inhibition	20	1000	6.11 ± 0.96	2.29 ± 0.42	5.95 ± 1.00	4.91 ± 0.18	11.42 ± 5.06	2.25 ± 0.31	4.59 ± 0.84	5.97 ± 0.47	3.06 ± 0.23	2.30 ± 0.16
	50	1000	3.22 ± 0.57	2.46 ± 0.38	2.99 ± 0.45	4.50 ± 0.17	8.04 ± 2.56	1.74 ± 0.21	2.64 ± 0.42	5.74 ± 0.32	2.59 ± 0.26	2.35 ± 0.10
	100	1000	2.04 ± 0.38	2.38 ± 0.35	2.14 ± 0.31	4.01 ± 0.17	6.09 ± 4.63	1.43 ± 0.19	1.94 ± 0.25	5.99 ± 0.47	1.84 ± 0.24	2.36 ± 0.13
Toxicity Detection	20	1000	5.95 ± 0.73	4.97 ± 0.31	5.03 ± 0.81	4.82 ± 0.09	11.26 ± 5.18	5.29 ± 0.29	5.27 ± 0.75	7.19 ± 0.44	6.71 ± 0.23	2.34 ± 0.15
	50	1000	4.03 ± 0.68	4.79 ± 0.26	<u>2.88 ± 0.48</u>	4.65 ± 0.08	8.75 ± 1.66	4.57 ± 0.30	3.37 ± 0.41	7.26 ± 0.47	5.38 ± 0.28	2.22 ± 0.13
	100	1000	2.43 ± 0.41	4.46 ± 0.22	1.90 ± 0.31	4.46 ± 0.11	7.41 ± 0.16	3.78 ± 0.26	2.34 ± 0.26	7.50 ± 0.60	3.80 ± 0.32	<u>2.14 ± 0.15</u>

Table S3: **Mean absolute error in accuracy estimation on binary tasks.** We report mean absolute error (MAE, averaging across classifiers) across five binary classification tasks and different amounts of labeled data. Each entry corresponds to the mean MAE across 50 randomized splits of data, accompanied by the 95% CI (computed as $1.96 \times$ the standard error) in MAE across splits. We bold the best performing method in each row, and underline the next best performing method by mean MAE. SSME-M refers to performance when fitting SSME to a single classifier's scores, instead of modeling the joint distribution of $P(y, s)$.

Dataset	n_ℓ	n_u	Labeled	Majority-Vote	PL	Dawid-Skene	SPE	BC	SSME-M	SSME (Ours)
Critical Outcome	20	1000	11.01 ± 1.12	2.75 ± 0.26	6.94 ± 0.64	<u>2.61 ± 0.09</u>	16.17 ± 6.69	3.48 ± 0.76	3.17 ± 0.30	1.16 ± 0.13
	50	1000	6.22 ± 0.62	3.68 ± 0.34	5.38 ± 0.39	<u>2.37 ± 0.09</u>	20.91 ± 9.43	2.56 ± 0.44	3.01 ± 0.26	1.13 ± 0.13
	100	1000	4.20 ± 0.38	3.43 ± 0.28	3.63 ± 0.21	2.25 ± 0.10	12.84 ± 8.93	<u>1.69 ± 0.25</u>	2.81 ± 0.22	1.15 ± 0.10
ED Revisit	20	1000	8.37 ± 0.87	<u>1.81 ± 0.02</u>	4.16 ± 0.82	3.25 ± 0.68	14.15 ± 10.31	3.57 ± 0.77	1.88 ± 0.24	0.76 ± 0.04
	50	1000	4.82 ± 0.48	<u>1.77 ± 0.03</u>	2.29 ± 0.47	2.29 ± 0.46	17.12 ± 7.09	2.04 ± 0.46	1.83 ± 0.19	0.73 ± 0.05
	100	1000	3.29 ± 0.24	1.69 ± 0.04	1.36 ± 0.22	1.34 ± 0.21	10.85 ± 4.82	<u>1.16 ± 0.20</u>	1.51 ± 0.17	0.73 ± 0.06
Hospital Admission	20	1000	21.76 ± 1.16	21.73 ± 2.75	8.10 ± 1.28	17.31 ± 0.13	16.79 ± 0.58	<u>5.12 ± 1.09</u>	5.54 ± 0.36	1.97 ± 0.13
	50	1000	12.74 ± 0.62	21.03 ± 2.65	5.02 ± 0.68	16.60 ± 0.13	14.87 ± 0.47	<u>3.49 ± 0.57</u>	5.20 ± 0.33	2.06 ± 0.18
	100	1000	8.56 ± 0.38	19.97 ± 2.45	3.91 ± 0.49	15.62 ± 0.13	13.39 ± 0.79	<u>3.23 ± 0.47</u>	5.32 ± 0.37	1.70 ± 0.15
SARS-CoV Inhibition	20	1000	7.44 ± 0.95	1.74 ± 0.38	5.96 ± 0.87	4.35 ± 0.15	11.85 ± 5.63	<u>2.24 ± 0.33</u>	2.57 ± 0.18	3.38 ± 0.13
	50	1000	3.66 ± 0.50	<u>1.96 ± 0.39</u>	3.06 ± 0.35	4.08 ± 0.16	8.96 ± 2.74	1.73 ± 0.26	2.27 ± 0.20	3.41 ± 0.11
	100	1000	2.18 ± 0.32	1.83 ± 0.37	2.36 ± 0.22	3.67 ± 0.16	7.28 ± 4.71	1.35 ± 0.22	<u>1.79 ± 0.19</u>	3.44 ± 0.13
Toxicity Detection	20	1000	5.85 ± 0.80	5.08 ± 0.39	5.09 ± 0.79	<u>4.40 ± 0.09</u>	11.23 ± 5.14	4.69 ± 0.34	5.67 ± 0.19	2.35 ± 0.13
	50	1000	3.99 ± 0.63	4.84 ± 0.33	<u>3.04 ± 0.46</u>	4.20 ± 0.07	7.97 ± 1.76	3.97 ± 0.34	4.57 ± 0.26	2.26 ± 0.12
	100	1000	2.37 ± 0.37	4.63 ± 0.33	1.91 ± 0.27	4.10 ± 0.09	6.75 ± 0.15	3.30 ± 0.25	3.43 ± 0.29	<u>2.19 ± 0.15</u>

Table S4: **Mean absolute error in ECE estimation on binary tasks.**

Dataset	n_ℓ	n_u	Labeled	Majority-Vote	PL	Dawid-Skene	SPE	BC	SSME-M	SSME (Ours)
Critical Outcome	20	1000	10.09 ± 1.34	9.45 ± 0.39	31.73 ± 1.10	9.39 ± 0.35	10.92 ± 4.41	<u>2.84 ± 0.25</u>	4.72 ± 0.63	2.52 ± 0.34
	50	1000	7.50 ± 1.28	8.06 ± 0.53	27.33 ± 1.53	8.49 ± 0.40	20.24 ± 11.78	<u>3.17 ± 0.32</u>	5.61 ± 1.28	2.39 ± 0.48
	100	1000	5.65 ± 0.95	7.29 ± 0.61	20.43 ± 1.22	7.97 ± 0.30	13.71 ± 10.26	2.70 ± 0.26	3.82 ± 0.48	<u>2.83 ± 0.80</u>
ED Revisit	20	1000	18.48 ± 1.85	19.99 ± 2.44	<u>7.48 ± 0.20</u>	8.27 ± 1.05	25.84 ± 6.42	7.65 ± 0.15	11.89 ± 1.29	5.92 ± 0.87
	50	1000	17.37 ± 1.98	17.93 ± 2.58	7.48 ± 0.26	7.62 ± 0.28	29.83 ± 4.67	<u>7.30 ± 0.21</u>	11.99 ± 1.21	5.09 ± 0.71
	100	1000	14.13 ± 1.67	14.95 ± 2.29	<u>7.06 ± 0.40</u>	7.09 ± 0.42	27.00 ± 3.59	7.47 ± 0.32	11.28 ± 1.59	5.08 ± 0.77
Hospital Admission	20	1000	6.97 ± 1.29	16.20 ± 1.00	8.94 ± 1.65	16.70 ± 0.10	15.81 ± 0.33	<u>2.67 ± 0.32</u>	3.63 ± 0.54	2.51 ± 0.38
	50	1000	5.08 ± 0.97	15.47 ± 0.56	5.59 ± 1.20	16.18 ± 0.10	14.93 ± 0.40	<u>2.62 ± 0.46</u>	3.18 ± 0.54	2.51 ± 0.33
	100	1000	3.57 ± 0.71	14.78 ± 0.44	3.66 ± 0.74	15.32 ± 0.12	13.95 ± 0.72	<u>2.55 ± 0.37</u>	3.17 ± 0.44	2.02 ± 0.33
SARS-CoV Inhibition	20	1000	9.61 ± 2.56	5.44 ± 0.60	30.92 ± 1.21	7.50 ± 0.29	13.72 ± 5.03	3.07 ± 0.28	5.42 ± 0.73	3.48 ± 0.44
	50	1000	5.84 ± 1.01	5.22 ± 0.39	22.71 ± 1.19	7.06 ± 0.29	10.67 ± 2.28	<u>3.62 ± 0.27</u>	5.02 ± 0.52	3.41 ± 0.47
	100	1000	3.97 ± 0.55	4.95 ± 0.35	16.33 ± 0.91	6.04 ± 0.32	10.34 ± 4.18	<u>3.53 ± 0.38</u>	4.21 ± 0.53	3.46 ± 0.45
Toxicity Detection	20	1000	6.71 ± 0.99	5.45 ± 0.82	17.32 ± 2.08	6.20 ± 0.11	12.38 ± 5.76	<u>5.22 ± 0.16</u>	6.05 ± 0.28	3.34 ± 0.23
	50	1000	4.76 ± 0.91	5.15 ± 0.47	11.79 ± 1.78	5.97 ± 0.09	8.23 ± 1.65	4.76 ± 0.21	4.86 ± 0.29	3.15 ± 0.18
	100	1000	<u>3.82 ± 0.60</u>	4.85 ± 0.20	7.54 ± 1.03	5.84 ± 0.12	7.28 ± 0.22	4.25 ± 0.27	4.15 ± 0.33	3.09 ± 0.22

Table S5: **Mean absolute error in AUC estimation on binary tasks.**

Dataset	n_ℓ	n_u	Labeled	Majority-Vote	PL	Dawid-Skene	SPE	BC	SSME-M	SSME (Ours)
Critical Outcome	20	1000	32.86 ± 5.06	36.21 ± 2.09	22.98 ± 1.85	39.02 ± 1.18	45.09 ± 6.81	<u>9.29 ± 1.67</u>	11.48 ± 1.51	6.11 ± 0.73
	50	1000	22.81 ± 3.65	26.12 ± 2.77	20.48 ± 2.23	35.64 ± 1.61	44.67 ± 7.31	<u>9.34 ± 1.43</u>	11.98 ± 1.43	6.17 ± 0.96
	100	1000	15.71 ± 2.44	24.01 ± 2.47	14.45 ± 2.02	33.31 ± 1.20	47.35 ± 6.71	<u>8.96 ± 1.41</u>	11.30 ± 1.67	5.77 ± 0.77
ED Revisit	20	1000	19.18 ± 3.68	<u>4.53 ± 1.59</u>	5.14 ± 0.89	5.12 ± 1.30	16.66 ± 11.60	9.14 ± 1.04	5.07 ± 0.80	1.67 ± 0.29
	50	1000	8.85 ± 2.26	3.12 ± 0.79	<u>2.72 ± 0.62</u>	3.04 ± 0.78	24.55 ± 10.06	6.03 ± 0.82	3.79 ± 0.65	1.81 ± 0.30
	100	1000	6.34 ± 1.54	3.23 ± 0.82	1.57 ± 0.33	<u>1.74 ± 0.34</u>	24.75 ± 12.17	4.23 ± 0.55	3.92 ± 0.62	1.82 ± 0.31
Hospital Admission	20	1000	9.43 ± 1.62	32.72 ± 6.41	10.89 ± 2.59	21.15 ± 0.16	21.13 ± 0.34	5.26 ± 1.07	<u>4.36 ± 0.44</u>	3.47 ± 0.57
	50	1000	7.46 ± 1.31	31.37 ± 6.28	7.91 ± 1.63	20.34 ± 0.18	19.21 ± 0.80	4.43 ± 0.74	<u>3.70 ± 0.63</u>	3.64 ± 0.60
	100	1000	5.51 ± 0.97	29.71 ± 5.98	4.12 ± 1.02	19.17 ± 0.21	18.73 ± 0.71	<u>3.49 ± 0.60</u>	4.00 ± 0.61	2.80 ± 0.51
SARS-CoV Inhibition	20	1000	22.27 ± 3.03	18.75 ± 2.82	37.41 ± 2.44	16.60 ± 1.08	41.22 ± 6.90	7.54 ± 0.76	13.81 ± 1.53	20.51 ± 1.70
	50	1000	15.02 ± 2.43	14.10 ± 1.05	30.29 ± 2.61	15.01 ± 1.07	34.97 ± 1.49	8.40 ± 0.96	<u>12.82 ± 1.01</u>	21.06 ± 1.51
	100	1000	11.53 ± 1.56	15.72 ± 2.66	20.34 ± 1.79	12.61 ± 1.05	33.60 ± 2.49	8.27 ± 0.89	<u>11.01 ± 1.39</u>	20.67 ± 1.64
Toxicity Detection	20	1000	19.34 ± 2.34	29.05 ± 3.31	25.12 ± 3.52	26.34 ± 0.36	37.10 ± 6.70	19.94 ± 1.30	23.38 ± 0.73	10.89 ± 0.87
	50	1000	<u>13.78 ± 1.81</u>	30.54 ± 3.70	20.15 ± 3.48	25.24 ± 0.36	31.94 ± 1.07	16.84 ± 1.58	18.90 ± 1.08	9.91 ± 0.85
	100	1000	<u>10.69 ± 1.71</u>	23.87 ± 0.84	14.06 ± 2.00	24.51 ± 0.47	30.94 ± 0.58	14.15 ± 1.48	14.59 ± 1.26	9.88 ± 0.97

Table S6: **Mean absolute error in AUPRC estimation on binary tasks.**

model	Labeled	Majority-Vote	PL	Dawid-Skene	SPE	BC	AutoEval	Active-Testing	SSME (Ours)	Ground Truth
distilbert-CORAL	83.90 ± 14.04	83.81 ± 13.35	86.15 ± 8.05	84.75 ± 2.64	73.48 ± 51.60	87.82 ± 8.64	85.04 ± 10.63	87.92 ± 21.20	86.49 ± 2.07	88.27 ± 0.18
distilbert-ERM	89.30 ± 12.04	91.34 ± 7.53	86.92 ± 6.57	95.08 ± 1.94	84.55 ± 51.41	97.13 ± 1.88	90.79 ± 11.63	89.17 ± 16.14	93.59 ± 1.71	92.17 ± 0.14
distilbert-ERM-seed1	89.10 ± 13.96	91.28 ± 7.50	87.05 ± 6.54	94.86 ± 2.06	93.25 ± 10.36	97.14 ± 1.97	90.75 ± 12.08	95.07 ± 12.69	93.54 ± 1.63	92.17 ± 0.15
distilbert-ERM-seed2	89.20 ± 12.42	91.63 ± 7.32	86.67 ± 6.72	95.78 ± 1.84	85.49 ± 46.57	96.28 ± 2.42	90.43 ± 13.38	92.84 ± 12.24	93.65 ± 1.61	92.11 ± 0.15
distilbert-IRM	86.90 ± 14.93	92.67 ± 9.76	82.92 ± 6.39	95.27 ± 1.29	93.48 ± 14.96	94.56 ± 4.59	88.11 ± 14.15	88.10 ± 17.89	91.65 ± 1.91	88.13 ± 0.18
distilbert-IRM-seed1	88.10 ± 14.40	92.87 ± 8.98	83.86 ± 6.49	95.92 ± 1.32	95.76 ± 12.55	95.41 ± 3.44	89.27 ± 13.77	89.42 ± 17.90	92.26 ± 1.65	89.04 ± 0.19
distilbert-IRM-seed2	86.80 ± 13.54	92.48 ± 9.09	83.39 ± 6.35	95.55 ± 1.35	86.76 ± 52.55	95.34 ± 4.27	87.78 ± 13.98	89.19 ± 18.15	92.08 ± 1.78	88.70 ± 0.16

Table S7: Mean absolute error in accuracy estimation per classifier on toxicity detection. .

model	Labeled	Majority-Vote	PL	Dawid-Skene	SPE	BC	SSME (Ours)	Ground Truth
distilbert-CORAL	13.80 ± 11.38	12.60 ± 9.19	8.78 ± 7.05	10.78 ± 2.12	25.34 ± 53.26	7.47 ± 8.12	8.50 ± 1.87	5.98 ± 0.18
distilbert-ERM	10.37 ± 11.48	8.16 ± 7.77	11.33 ± 6.44	4.37 ± 2.08	14.87 ± 49.40	1.97 ± 1.97	4.96 ± 1.47	6.14 ± 0.17
distilbert-ERM-seed1	9.91 ± 12.33	8.34 ± 7.65	11.29 ± 6.35	4.59 ± 2.21	6.45 ± 10.72	1.93 ± 2.09	5.13 ± 1.53	6.21 ± 0.16
distilbert-ERM-seed2	10.02 ± 11.80	7.70 ± 7.75	10.96 ± 6.53	3.38 ± 1.93	14.36 ± 46.44	2.32 ± 2.47	3.99 ± 1.39	4.94 ± 0.19
distilbert-IRM	12.59 ± 13.50	6.52 ± 9.97	15.77 ± 6.04	3.69 ± 1.31	6.69 ± 14.92	4.61 ± 5.14	6.85 ± 1.72	10.61 ± 0.16
distilbert-IRM-seed1	11.93 ± 13.31	6.35 ± 9.18	15.03 ± 6.38	2.98 ± 1.24	4.18 ± 12.63	3.88 ± 3.89	6.38 ± 1.83	9.78 ± 0.21
distilbert-IRM-seed2	12.06 ± 12.00	6.71 ± 9.42	15.55 ± 6.16	3.33 ± 1.46	13.01 ± 51.77	3.87 ± 4.60	6.71 ± 1.74	10.18 ± 0.18

Table S8: Mean absolute error in ECE estimation per classifier on toxicity detection.

model	Labeled	Majority-Vote	PL	Dawid-Skene	SPE	BC	SSME (Ours)	Ground Truth
distilbert-CORAL	85.19 ± 27.74	90.53 ± 8.91	72.20 ± 13.51	94.89 ± 2.31	79.61 ± 72.95	84.22 ± 6.84	91.38 ± 3.14	86.23 ± 0.33
distilbert-ERM	91.80 ± 13.93	96.36 ± 8.70	74.90 ± 15.08	98.64 ± 0.65	90.62 ± 57.77	98.52 ± 1.84	95.97 ± 1.50	93.77 ± 0.22
distilbert-ERM-seed1	92.18 ± 14.63	96.36 ± 8.76	74.92 ± 15.05	98.58 ± 0.59	99.70 ± 0.58	98.30 ± 1.86	95.96 ± 1.39	93.75 ± 0.20
distilbert-ERM-seed2	93.32 ± 11.62	96.55 ± 8.86	75.03 ± 15.17	98.89 ± 0.62	90.81 ± 57.23	98.07 ± 2.20	96.16 ± 1.33	94.08 ± 0.19
distilbert-IRM	91.46 ± 17.13	95.52 ± 13.36	74.69 ± 14.67	98.28 ± 1.17	99.06 ± 3.55	98.05 ± 1.88	95.38 ± 2.22	91.57 ± 0.25
distilbert-IRM-seed1	90.75 ± 20.55	95.25 ± 12.97	74.58 ± 14.85	97.97 ± 1.60	99.52 ± 1.60	98.07 ± 2.00	95.18 ± 2.19	91.00 ± 0.31
distilbert-IRM-seed2	91.89 ± 15.94	95.37 ± 13.62	74.68 ± 14.90	98.39 ± 1.02	90.44 ± 57.04	98.33 ± 1.84	95.59 ± 1.79	91.86 ± 0.23

Table S9: Mean absolute error in AUC estimation per classifier on toxicity detection.

model	Labeled	Majority-Vote	PL	Dawid-Skene	SPE	BC	SSME (Ours)	Ground Truth
distilbert-CORAL	60.78 ± 47.30	67.66 ± 48.12	31.91 ± 19.96	76.38 ± 9.81	71.94 ± 75.73	50.86 ± 21.03	60.27 ± 10.78	40.00 ± 0.70
distilbert-ERM	77.25 ± 38.26	82.78 ± 55.03	42.28 ± 26.91	94.59 ± 2.39	79.50 ± 71.95	92.51 ± 8.47	79.63 ± 7.22	72.19 ± 0.73
distilbert-ERM-seed1	79.38 ± 36.73	83.34 ± 53.48	42.27 ± 26.76	94.37 ± 2.25	83.36 ± 69.87	91.54 ± 9.68	79.78 ± 6.78	72.30 ± 0.68
distilbert-ERM-seed2	79.11 ± 35.38	83.41 ± 55.47	42.47 ± 27.03	95.49 ± 2.34	78.44 ± 73.38	90.15 ± 9.69	80.06 ± 6.54	73.33 ± 0.69
distilbert-IRM	77.74 ± 38.16	81.26 ± 57.61	40.79 ± 25.87	92.89 ± 2.88	81.71 ± 76.90	88.23 ± 14.48	76.90 ± 8.27	65.86 ± 0.78
distilbert-IRM-seed1	79.21 ± 39.17	81.73 ± 57.61	41.23 ± 26.40	93.64 ± 3.17	82.29 ± 74.37	89.58 ± 11.12	77.84 ± 7.67	66.50 ± 0.86
distilbert-IRM-seed2	77.63 ± 39.97	80.53 ± 57.24	40.65 ± 26.19	92.67 ± 3.46	77.63 ± 77.91	90.34 ± 12.47	77.16 ± 7.20	65.46 ± 0.79

Table S10: Mean absolute error in AUPRC estimation per classifier on toxicity detection.

Dataset	n_ℓ	n_u	Labeled	Majority-Vote	PL	Dawid-Skene	AutoEval	Active-Testing	SSME (Ours)
AG News	20	1000	5.48 ± 0.89	5.13 ± 0.16	11.72 ± 1.23	6.70 ± 0.13	5.59 ± 1.18	8.09 ± 0.80	3.72 ± 0.19
	50	1000	3.92 ± 0.63	4.96 ± 0.14	5.22 ± 0.78	6.51 ± 0.12	4.36 ± 0.78	8.88 ± 1.40	3.54 ± 0.17
	100	1000	2.71 ± 0.45	4.74 ± 0.19	2.69 ± 0.48	6.20 ± 0.16	2.71 ± 0.59	8.77 ± 1.20	3.41 ± 0.24
MultiNLI	20	1000	7.46 ± 1.07	8.30 ± 0.35	7.95 ± 1.26	11.73 ± 0.15	7.20 ± 1.04	10.30 ± 1.77	1.98 ± 0.24
	50	1000	4.42 ± 0.55	8.14 ± 0.27	3.08 ± 0.62	11.41 ± 0.14	4.17 ± 0.54	11.85 ± 1.70	1.90 ± 0.21
	100	1000	3.27 ± 0.46	7.54 ± 0.30	2.47 ± 0.51	10.72 ± 0.15	3.17 ± 0.44	11.63 ± 1.77	2.02 ± 0.23

Table S11: Mean absolute error in accuracy estimation on multiclass tasks.

Dataset	n_ℓ	n_u	Labeled	Majority-Vote	PL	Dawid-Skene	SSME (Ours)
AG News	20	1000	5.53 ± 0.93	4.30 ± 0.13	11.85 ± 1.21	5.80 ± 0.11	3.37 ± 0.17
	50	1000	3.88 ± 0.76	4.18 ± 0.11	5.36 ± 0.77	5.70 ± 0.10	3.28 ± 0.15
	100	1000	2.61 ± 0.49	4.07 ± 0.15	2.78 ± 0.48	5.53 ± 0.13	3.13 ± 0.21
MultiNLI	20	1000	11.57 ± 1.13	3.87 ± 0.18	7.84 ± 1.14	2.95 ± 0.08	2.06 ± 0.24
	50	1000	6.14 ± 0.67	3.94 ± 0.14	3.10 ± 0.62	2.92 ± 0.10	2.06 ± 0.20
	100	1000	4.52 ± 0.51	3.82 ± 0.15	2.37 ± 0.46	3.18 ± 0.08	2.19 ± 0.21

Table S12: Mean absolute error in ECE estimation on multiclass tasks.

model	SSME-KDE-gaussian	SSME-KDE-epanechnikov	SSME-KDE-exponential
distilbert_CORAL	86.61 ± 1.3587	86.61 ± 1.3586	86.60 ± 1.3884
distilbert_ERM	93.83 ± 1.0066	93.83 ± 1.0067	93.81 ± 0.9879
distilbert_ERM_seed1	93.76 ± 0.9585	93.75 ± 0.9584	93.73 ± 0.9314
distilbert_ERM_seed2	93.77 ± 0.6859	93.77 ± 0.6859	93.75 ± 0.6643
distilbert_IRM	91.80 ± 1.0459	91.80 ± 1.0460	91.78 ± 1.0122
distilbert_IRM_seed1	92.37 ± 1.0373	92.37 ± 1.0373	92.35 ± 1.0252
distilbert_IRM_seed2	92.33 ± 0.9593	92.33 ± 0.9592	92.31 ± 0.9346

Table S13: **Robustness of SSME to kernel choice.** Because density estimation can be sensitive to kernel choice, we analyze the stability of SSME’s performance estimates across three kernel types. We find no significant impact of kernel choice on SSME’s performance estimates (although different kernels do produce small changes in accuracy estimates). Results hold across metrics and tasks; we report results for each toxicity detection classifier and accuracy for brevity.

Dataset	n_ℓ	n_u	Labeled	Majority-Vote	PL	Dawid-Skene	AutoEval	Active-Testing	SSME (Ours)	SSME-NF
AG News	20	1000	5.48 ± 0.45	5.13 ± 0.08	11.72 ± 0.63	6.70 ± 0.07	5.59 ± 0.60	8.09 ± 0.41	3.72 ± 0.10	3.52 ± 0.11
	50	1000	3.92 ± 0.32	4.96 ± 0.07	5.22 ± 0.40	6.51 ± 0.06	4.36 ± 0.40	8.88 ± 0.72	3.54 ± 0.09	3.50 ± 0.11
	100	1000	2.71 ± 0.23	4.74 ± 0.10	2.69 ± 0.25	6.20 ± 0.08	2.71 ± 0.30	8.77 ± 0.61	3.41 ± 0.12	3.40 ± 0.13
MultiNLI	20	1000	7.46 ± 0.55	8.30 ± 0.18	7.95 ± 0.64	11.73 ± 0.08	7.20 ± 0.53	10.30 ± 0.90	1.98 ± 0.12	3.08 ± 0.09
	50	1000	4.42 ± 0.28	8.14 ± 0.14	3.08 ± 0.32	11.41 ± 0.07	4.17 ± 0.28	11.85 ± 0.87	1.90 ± 0.11	2.79 ± 0.11
	100	1000	3.27 ± 0.23	7.54 ± 0.15	2.47 ± 0.26	10.72 ± 0.08	3.17 ± 0.23	11.63 ± 0.90	2.02 ± 0.12	2.52 ± 0.11

Table S14: **Mean absolute error in accuracy estimation on multiclass tasks, including NF parametrization.** SSME-NF performs comparably or worse than SSME (Ours) across the two multiclass tasks and three labeled data settings we consider.

D.5 Results reporting performance of alternate parameterization

SSME can be fit using other functions to approximate $P(s|y)$. We additionally explored the value of parameterizing each component using a normalizing flow (implementation details in Sec. E.3), a technique that is increasingly used to approximate complex densities [2].

We find that using a KDE outperforms the normalizing flow on each binary task, for every metric (except estimating AUPRC for SARS-CoV inhibition prediction, Table S15). We find that the KDE performs similarly to the normalizing flow for each LLM-based task, although by a smaller margin (Table S14). We hypothesize that this is due to the established challenges of approximating multi-modal distributions with normalizing flows [65, 16].

For higher-dimensional tasks, the normalizing flow seems to outperform the KDE. In particular, we ran an experiment on ImagenetBG, which contains nine classes and four classifiers. Table S16 demonstrates that in this setting, the normalizing flow performs better than the KDE.

Dataset	n_ℓ	n_u	Labeled	SSME-M	SSME (Ours)	SSME-NF
Critical Outcome	20	1000	5.19 ± 1.07	1.70 ± 0.27	0.67 ± 0.13	9.80 ± 1.41
	50	1000	2.90 ± 0.59	1.65 ± 0.25	0.78 ± 0.13	8.81 ± 1.11
	100	1000	2.09 ± 0.41	1.30 ± 0.20	0.77 ± 0.13	8.28 ± 1.64
ED Revisit	20	1000	5.11 ± 0.98	1.64 ± 0.34	0.45 ± 0.10	3.54 ± 1.87
	50	1000	2.02 ± 0.58	1.46 ± 0.27	0.53 ± 0.11	2.63 ± 1.10
	100	1000	1.43 ± 0.32	1.18 ± 0.25	0.57 ± 0.11	2.51 ± 0.94
Hospital Admission	20	1000	7.32 ± 1.25	3.29 ± 0.47	1.88 ± 0.29	3.19 ± 0.95
	50	1000	5.40 ± 0.83	3.17 ± 0.51	1.95 ± 0.27	2.27 ± 0.62
	100	1000	3.64 ± 0.55	3.06 ± 0.45	1.51 ± 0.23	3.66 ± 2.31
SARS-CoV Inhibition	20	1000	6.11 ± 0.96	3.06 ± 0.23	2.30 ± 0.16	11.67 ± 5.26
	50	1000	3.22 ± 0.57	2.59 ± 0.26	2.35 ± 0.10	20.89 ± 7.38
	100	1000	2.04 ± 0.38	1.84 ± 0.24	2.36 ± 0.13	9.89 ± 4.52
Toxicity Detection	20	1000	5.95 ± 0.73	6.71 ± 0.23	2.34 ± 0.15	3.44 ± 0.11
	50	1000	4.03 ± 0.68	5.38 ± 0.28	2.22 ± 0.13	3.31 ± 0.13
	100	1000	2.43 ± 0.41	3.80 ± 0.32	2.14 ± 0.15	3.32 ± 0.13

Table S15: **Mean absolute error in accuracy estimation on binary tasks, including NF parametrization.** We include columns for the Labeled, SSME fit to each classifier individually (SSME-M), SSME parameterized by a KDE (SSME (Ours)), and SSME parameterized by an NF (SSME-NF). While SSME-NF sometimes outperforms SSME-M, SSME-NF never outperforms SSME-KDE on accuracy estimation in any of the tasks or amounts of labeled data we consider.

Dataset	n_ℓ	n_u	Labeled	Majority-Vote	PL	DS	AutoEval	Active-Testing	SSME (KDE)	SSM
ImnetBG	20	1000	6.62 ± 2.74	2.99 ± 0.90	33.45 ± 2.96	5.78 ± 0.71	6.55 ± 2.62	10.83 ± 5.34	8.76 ± 1.00	2.65
ImnetBG	50	1000	3.98 ± 1.63	3.01 ± 0.61	17.88 ± 2.78	5.69 ± 0.73	3.87 ± 1.56	12.25 ± 7.28	8.18 ± 0.90	2.66
ImnetBG	100	1000	2.97 ± 1.38	2.73 ± 0.57	9.37 ± 1.53	5.34 ± 0.63	2.73 ± 1.13	9.08 ± 4.22	8.02 ± 0.90	2.10

Table S16: Comparison across evaluation methods on the *ImnetBG* dataset with varying numbers of labeled examples (n_ℓ) and unlabeled examples (n_u). SSME (NF) consistently achieves the lowest MAE.

Labeled Examples	Initialization	MAE, ECE	MAE, Accuracy
20	KNN	0.045	0.046
20	Draw	0.035	0.034
50	KNN	0.037	0.040
50	Draw	0.043	0.043
100	KNN	0.031	0.033
100	Draw	0.037	0.036

Table S17: Performance comparison across different numbers of labeled examples and initialization methods (Dataset: CivilComments).

D.6 Results reporting robustness to initializations

We find that SSME’s performance remains strong when using an alternative plausible initialization method: using a majority vote among $k=5$ nearest neighbors among the labeled examples to initialize cluster assignment for unlabeled examples. We compare this alternate initialization method to our original initialization method (which we refer to as “draw” in the table) on the CivilComments dataset with three different amounts of labeled data (20, 50, and 100 points). We include our results on ECE and accuracy estimation error in the table S17, where we find that the two initialization methods perform comparably on the CivilComments dataset.

D.7 Results reporting performance as number of classifiers increases

As shown in table S18, we find that SSME’s performance improves as the number of classifiers increases, which accords with our theoretical results. As a caveat, our theory predicts that SSME is likely not to perform well if one adds an inaccurate (e.g., worse than random) classifier to the set.

We also find that SSME’s performance does not vary greatly across classifier sets, suggesting that SSME’s performance is robust to using different classifier sets. In particular, the standard deviation in accuracy estimation error across random classifier sets is always under 0.011, and the standard deviation in ECE estimation error is always under 0.015, indicating consistent performance across classifier sets.

First, we find that performance does not vary greatly across classifier sets, suggesting that SSME’s performance is robust to using different classifiers. In particular, the standard deviation in accuracy estimation error across random classifier sets is always under 0.011, and the standard deviation in ECE estimation error is always under 0.015.

Second, we find that SSME’s performance improves as the number of classifiers increases, which accords with our theoretical results. As a caveat, our theory predicts that SSME is likely not to perform well if one adds an inaccurate (e.g., worse than random) classifier to the set.

D.8 Results reporting performance for different bandwidth selection procedures

We ran an experiment to test the robustness of our results to the choice of bandwidth. In the paper, we use the Sheather-Jones algorithm to automatically identify a bandwidth. We compare this approach to (1) another automated bandwidth selection algorithm (the Silverman algorithm) and (2) two fixed bandwidths, chosen to be larger but within an order of magnitude of the Sheather-Jones selected bandwidth. We conduct experiments using the CivilComments dataset and 3 labeled dataset sizes

# Classifiers	MAE, ECE (SD)	MAE, Accuracy (SD)
2	0.0457 (0.0059)	0.0471 (0.0047)
3	0.0302 (0.0107)	0.0308 (0.0098)
4	0.0268 (0.0094)	0.0273 (0.0096)
5	0.0252 (0.0072)	0.0253 (0.0078)
6	0.0235 (0.0043)	0.0235 (0.0048)
7	0.0225 (only one subset)	0.0223 (only one subset)

Table S18: Performance as the number of classifiers increases. Standard deviations (SD) are shown in parentheses. Dataset: CivilComments.

# Labeled Examples	Bandwidth Selection Procedure	MAE, ECE	MAE, Accuracy
20	Sheather-Jones	0.024	0.023
20	Silverman	0.040	0.038
20	1.0	0.037	0.036
20	2.0	0.046	0.044
50	Sheather-Jones	0.023	0.022
50	Silverman	0.066	0.065
50	1.0	0.062	0.062
50	2.0	0.045	0.044
100	Sheather-Jones	0.022	0.021
100	Silverman	0.049	0.047
100	1.0	0.056	0.055
100	2.0	0.034	0.032

Table S19: (Dataset: *CivilComments*) Comparison of bandwidth selection procedures. Sheather-Jones outperforms another automated selection method (Silverman) and two fixed bandwidths.

(20, 50, and 100 labeled datapoints). While results remain strong in all cases, we achieve the best performance when using the Sheather-Jones bandwidth selection procedure.

D.9 Comparison to baselines drawn from weak supervision

Popular approaches to weak supervision including Snorkel [58] and FlyingSquid [27] implement a latent variable model equivalent to Dawid-Skene. Both works build on Dawid-Skene to incorporate information about pairwise correlations between labeling functions; [58] employs a technique to infer dependencies, while [27] assume these dependencies to be user-provided. When we applied a standard approach to dependency inference [4] in our setting, we observed that (1) all classifiers are inferred to be dependent on one another, and (2) the number of dependencies raised issues with convergence. It is thus not feasible to incorporate dependency inference, and the resulting latent variable model is equivalent to Dawid-Skene.

D.10 Comparison to ensembling

While we limit the scope of our experiments in the main text to semi-supervised methods that make use of *both* labeled and unlabeled data, another approach would be to produce an estimate of $Pr(y = k | s^{(i)})$ by averaging the classifier scores. This approach results in an unbiased metric estimator when the resulting ensemble is calibrated, as theoretical results by [37] show. Such an approach has natural downsides: it is sensitive to the composition of the classifier set, does not improve with the introduction of labeled data, and relies on an assumption of ensemble calibration that is unlikely to hold in practice [71]. Here, we provide experiments to illustrate this behavior.

We use a semisynthetic setting to conduct a comparison to ensembling. To do so, we create sets of three classifiers based on the widely-used Adult dataset [7], where the task is to predict whether a person's income is above \$50K. To create differences between the three classifiers in a set, we train them on random fixed-size samples of 50 labeled examples from different portions of the dataset, partitioned based on age. In doing so, our semi-synthetic classifier sets mimic how training data for

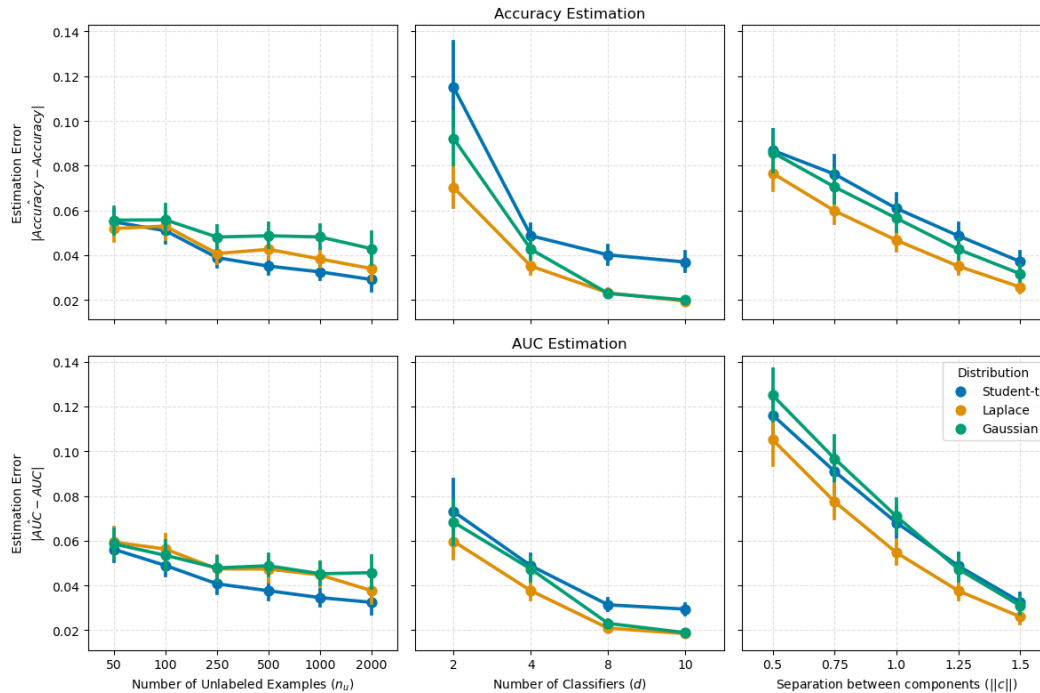


Figure S2: **SSME performance in response to additional unlabeled data, additional classifiers, and improved classifiers.** As indicated by our theoretical results, SSME benefits from increased amounts of unlabeled data, number of classifiers, and classifier performance.

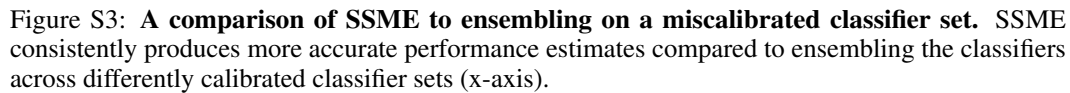
different real-world classifiers can differ in meaningful ways. We repeat this procedure to produce 500 sets of three classifiers, where sets differ in the training data provided to each classifier. Our procedure naturally produces random variation in classifier properties, like accuracy and calibration. As with the real datasets, we produce three splits: a training split to learn the classifiers (50 examples), an estimation split for the performance estimation methods (20 labeled examples and 1000 unlabeled examples), and an evaluation split to measure ground truth values for each metric (10,000 examples). Each classifier is a logistic regression with default L2 regularization.

We artificially increase the expected calibration error of each classifier using a generalized logistic function parameterized by a . Specifically, we transform classifier score s to be $\frac{s^a}{s^a + (1-s)^a}$, effectively increasing overconfidence for higher s and increasing underconfidence for lower s . As in the semisynthetic experiments, we generate 500 semisynthetic classifier sets, where each classifier in a set is trained on 100 examples distinct from the training data for other classifiers in the set (results are robust to this choice of training dataset size). Each set contains three classifiers.

Figure S3 reports our results. As the average calibration among classifiers in a set varies, SSME consistently improves over the use of an ensemble. This aligns with our intuition, and indicates the value of using labeled data in conjunction with unlabeled data. Miscalibration has little effect on the ensemble when estimating AUPRC; here, SSME and ensembling perform similarly.

D.11 Comparison of computational cost

Fitting SSME is computationally cheap and faster than the best baseline. For every dataset and experiment configuration reported in the paper, SSME can be fit in under 5 minutes, using only 1 CPU. SSME inherits the computational complexity of kernel density estimators ($O(n^2)$) and EM. In a matched comparison (using 20 labeled examples, 1000 unlabeled examples, and 7 classifiers) the next best-performing baseline (Bayesian-Calibration) takes on average 32.1 seconds to estimate performance, while SSME takes 21.5 seconds.



Input: Labeled set $\mathcal{D}_\ell = \{(\mathbf{s}^{(i)}, y^{(i)})\}_{i=1}^{n_\ell}$; Unlabeled set $\mathcal{D}_u = \{\mathbf{s}^{(i)}\}_{i=1}^{n_u}$; $\mathbf{s}^{(i)}$ are **ALR-transformed** classifier scores; Fitted model $P_\theta(y \mid \mathbf{s})$; metric function $g(\mathbf{p}, y)$;
Number of samples $S = 500$

E Method Details

Given a vector $p \in \Delta^{K-1}$ over K classes, let $\mathbf{s} = \text{ALR}(\mathbf{p}) = \left[\log \frac{\mathbf{p}_1}{\mathbf{p}_K}, \log \frac{\mathbf{p}_2}{\mathbf{p}_K}, \dots, \log \frac{\mathbf{p}_{K-1}}{\mathbf{p}_K} \right] \in \mathbb{R}^{K-1}$. To invert, $\mathbf{p}_i = \frac{e^{s_i}}{1 + \sum_{k=1}^{K-1} e^{s_k}}$ for $i < K$ and $\mathbf{p}_K = \frac{1}{1 + \sum_{k=1}^{K-1} e^{s_k}}$. The ALR transform maps unit-sum data into real space, where it is easier to fit mixture models. The inverse allows us to map samples from the mixture model in real space back to the simplex Δ^{K-1} . For details, see [53].

SSME is able to estimate any metric that is a function of the classifier probabilities p and label y . We approximate the joint distribution $P(y, \mathbf{p})$ with a mixture model $P_{\theta}(y, \mathbf{s})$, where $\mathbf{s}$ refers to the ALR-transformed classifier probabilities (i.e. “classifier scores”)². We refer to $P(y, \mathbf{p})$ for ease of notation in this section; it is equivalent, through invertible mapping, to $P(y, \mathbf{s})$.

²Recall that ALR is a bijection, so we use the inverse mapping $\text{ALR}^{-1} : \mathbb{R}^{K-1} \rightarrow \Delta^{K-1}$ to transform our mixture distribution in real space back to probability space.

Accuracy measures the alignment between a model's (discrete) predictions and the true label y . To discretize predictions, practitioners typically take the argmax of $\mathbf{p}^{(i)}$. Using the binary case an illustrative example, the accuracy of the j th model can be written as:

$$\text{Accuracy}_j = \mathbb{E}_{\mathbf{p}} [\mathbf{1}[y = \mathbf{1}(\mathbf{p} > t)]]$$

where $\mathbf{1}$ is an indicator function and t is a chosen threshold, typically 0.5. In our setting, we approximate this as:

$$\text{Accuracy}_j \approx \frac{1}{n_u + n_\ell} \sum_{i=1}^{n_u + n_\ell} \mathbf{1}[y^{(i)} = \mathbf{1}(\mathbf{p}^{(i)} > t)]$$

For labeled examples, we use the true label $y^{(i)}$. For unlabeled examples, we draw $y^{(i)} \sim P_\theta(y|\mathbf{p}^{(i)})$. We then compute accuracy using these labels $y^{(i)}$ and predictions $\mathbf{p}^{(i)}$. To ensure our estimation procedure is robust to sampling noise, we average our estimated accuracy over 500 separate sampled labels for each example in the unlabeled dataset.

Alternatively, we could directly use $P_\theta(y|\mathbf{p})$ to estimate accuracy. That is, for each point $\mathbf{p}^{(i)}$ we directly compute an expectation for the label, and sum this over the entire dataset.

Using the binary case as an example

$$\text{Accuracy}_j \approx \frac{1}{n_u + n_\ell} \sum_{i=1}^{n_u + n_\ell} \mathbb{E} [\mathbf{1}[y^{(i)} = \mathbf{1}(\mathbf{p}_j^{(i)} > t)] | \mathbf{p}^{(i)}]$$

In other words, we compute the expectation that the true label agrees with the predicted label for each point. This expectation is $\mathbf{p}^{(i)}$. This expectation is computed over $P_\theta(y|\mathbf{p})$. One can interpret $P_\theta(y|\mathbf{p})$ as a "recalibration" step: given a set of classifier guesses $\mathbf{p}$, what is the true distribution of y ?

In our experiments, we use the first of these two approaches, i.e. we sample the true label from the estimated distribution.

Expected Calibration Error (ECE) measures the alignment between a model's predicted probabilities $\mathbf{p}_j$ and the ground truth labels y . In particular, ECE compares the model's reported confidence to the true class likelihoods, averaged over the dataset. We write out our ECE estimation procedure for the binary case, and it extends readily to definitions of calibration in multiclass settings [32]. Binary ECE can be written as:

$$\text{ECE}_j = \mathbb{E}_{\mathbf{p}_j} \left[\left| P(\hat{Y} = 1 | \hat{p} = \mathbf{p}_j) - \mathbf{p}_j \right| \right]$$

Then, to approximate the ECE with the datasets $\{\mathbf{p}^i\}_{i=1}^{n_u}$ and $\{\mathbf{p}^i, y^{(i)}\}_{i=1}^{n_\ell}$, one can sample $y^{(i)} \sim P_\theta(y|\mathbf{p}^{(i)})$ for each unlabeled sample i and then use the standard histogram binning procedure [31] using both the true labels for the labeled dataset and the sampled labels for the unlabeled dataset. In this approach, we treat the sampled labels $y^{(i)}$ as true labels for unlabeled examples. To ensure our procedure is robust against sampling noise, we draw samples of $y^{(i)}$ repeatedly for a fixed number of draws (500). We then compute ECE separately for each of these 500 draws and average ECE across all draws.

We use this first approach, but alternatively, one could also *directly* use $P_\theta(y|\mathbf{p})$ to estimate ECE. In particular, we can write:

$$\text{ECE}_j \approx \frac{1}{n_u + n_\ell} \sum_{i=1}^{n_u + n_\ell} \left| P_\theta(y = 1 | \mathbf{p}_j^{(i)}) - \mathbf{p}_j^{(i)} \right|$$

In this approach, we don't sample the labels y for unlabeled examples but instead directly use $P_\theta(y|\mathbf{p})$, which provides us (an estimate of) the true distribution of y . Instead, we directly use our estimate for the conditional label distribution $P_\theta(y = 1 | \mathbf{p}_j^{(i)})$.

In our experiments, we use the first approach described, i.e. sampling $y^{(i)}$ for unlabeled examples and then using the standard binning and averaging procedure.

AUROC and AUPRC can be estimated with a similar procedure as above. In particular, we sample a label $y^{(i)} \sim P_\theta(y = 1|\mathbf{p}^{(i)})$ from the conditional label distribution and compare these sampled labels to the classifier probabilities.

E.3 Alternate parameterizations

One alternative parameterization is to use a normalizing flow to model our mixture of distributions. Normalizing flows learn and apply an invertible transform f_θ to a random variable $\mathbf{z} \sim D_1$ to obtain $f_\theta(\mathbf{z}) \sim D_2$. Here, we set $\mathbf{z} \sim D_1$ to a Gaussian mixture model and learn a transformation such that $f_\theta(\mathbf{z}) \stackrel{\text{dist.}}{\approx} \mathbf{s}$, i.e., the transformed distribution roughly matches our classifier score distribution. By modeling $\mathbf{z}$ explicitly as a Gaussian mixture model, one can move back and forth between the two distributions, as $f_\theta^{-1}(f_\theta(\mathbf{z})) = \mathbf{z}$, where f_θ^{-1} is the inverse of f . Specifically, we set the distribution of $\mathbf{Z}$ to follow a Gaussian mixture:

$$\mathbf{Z}|(Y = k) \sim \mathcal{N}(\mu_k, \Sigma_k)$$

Thus, the marginal distribution of $\mathbf{Z}$ is $p_{\mathbf{Z}}(\mathbf{z}) = \sum_{k=1}^K \mathcal{N}(\mathbf{z}|\mu_k, \Sigma_k) \cdot p(y = k)$ is the overall density of $\mathbf{z}$. We apply our invertible transformation f_θ to obtain $\mathbf{s} = f_\theta(\mathbf{z})$. To find $p(\mathbf{s}|y = k)$, we follow the approach of [35]:

$$p_{\mathbf{S}}(\mathbf{s}|y = k) = \mathcal{N}(f_\theta^{-1}(\mathbf{s})|\mu_k, \Sigma_k) \cdot \left| \det \left(\frac{\delta f}{\delta x} \right) \right| \cdot p(y = k)$$

Intuitively, we transform $(\mathbf{s}, y)$ into a distribution $(\mathbf{z}, y)$ which follows a Gaussian mixture model. By enforcing the constraint that this transform is invertible, the joint distribution on $(\mathbf{z}, y)$ captures all the information in $(\mathbf{s}, y)$.

We use the RealNVP architecture [22] to parameterize f_θ using 10 coupling layers, 3 fully-connected layers, and a hidden dimension of 128 between the fully connected layers. Our normalizing flow is lightweight and trains in less than a minute for each dataset in our experiments section using 1 80GB NVIDIA A100 GPU.

Note there are two optimizations here: (1) the normalizing flow transformation f_θ which maps $\mathbf{s}$ into our latent Gaussian mixture space and (2) the Gaussian mixture model parameters μ_k, Σ_k themselves. We begin by fixing the GMM parameters μ_k, Σ_k to values estimated from our classifier scores $\mathbf{s}$ and learning only the flow f_θ for 300 epochs. Afterwards, we optimize the GMM parameters μ_k, Σ_k with EM for another 700 epochs.