KNOWLEDGE DISTILLATION AS SEMIPARAMETRIC INFERENCE

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ABSTRACT

A popular approach to model compression is to train an inexpensive student model to mimic the class probabilities of a highly accurate but cumbersome teacher model. Surprisingly, this two-step knowledge distillation process often leads to higher accuracy than training the student directly on labeled data. To explain and enhance this phenomenon, we cast knowledge distillation as a semiparametric inference problem with the optimal student model as the target, the unknown Bayes class probabilities as nuisance, and the teacher probabilities as a plug-in nuisance estimate. By adapting modern semiparametric tools, we derive several new guarantees for the prediction error of standard distillation and develop several enhancements with improved guarantees. We validate our findings empirically on both tabular data and image data and observe consistent improvements from our knowledge distillation enhancements.

1 INTRODUCTION

Knowledge distillation (KD) (Craven & Shavlik, 1996; Breiman & Shang, 1996; Bucila et al., 2006; Li et al., 2014; Ba & Caruana, 2014; Hinton et al., 2015) is a widely used model compression technique that enables deployment of ML models on devices such as phones, watches, and virtual assistants (Stock et al., 2020). KD works by training a large teacher model and then a smaller student model that tries to match the teacher's predictions. It is easily applied to any classification procedure and any teacher and works remarkably well across a wide variety of domains including computer vision (Hinton et al., 2015), natural language processing (Sanh et al., 2019), and tabular data settings (Liu et al., 2018; Tan et al., 2018; Fakoor et al., 2020). Despite KD's ubiquity and importance, the reasons for its success remains elusive. The practice of KD is often guided by heuristics.

In practice, KD is often performed in diverse ways, for different tasks and different domains. It is often tailored to particular model types (e.g., CNN, RNNs, Transformer). This precludes a general theoretical understanding of KD. Hinton et al. (2015) remarks that KD works by transferring the "dark knowledge" from the teacher's predicted class probabilities. As we detail below, several works have tried to explain how this dark knowledge can improve the student's performance beyond training from scratch. Our work is motivated by the observation of Menon et al. (2020) that the teacher probabilities serve as a proxy for the *Bayes probabilities* (i.e., the true class probabilities) and that the closer the teacher and Bayes probabilities, the better the student's performance should be.

Building on this observation, we cast KD as a plug-in approach to *semiparametric inference*: distillation aims to fit a student model $\hat{f}$ in the presence of nuisance (the Bayes probabilities p_0) with the teacher's probabilities $\hat{p}$ as a plug-in estimate of p_0. This insight allows us to adapt modern tools from semiparametric inference to analyze the error of a distilled student in Sec. 3. Our analysis further suggests several enhancements for KD. For example, in Sec. 4 we show that avoiding sample reuse between the teacher and student through *cross-fitting* (see, e.g., Chernozhukov et al., 2018) can improve KD performance. Moreover, a common strategy in semiparametric inference is to improve plug-in estimation by reducing plug-in bias. The method of *orthogonal machine learning* (Chernozhukov et al., 2018; Foster & Syrgkanis, 2019) suggests correcting the teacher's probabilities by stepping in the $y-\hat{p}$ direction where y is an observed label vector. We argue in Sec. 4 that while this minimizes the teacher bias, the variance could explode. We instead propose a correction that balances the bias and variance, leading to a better overall generalization bound.

We empirically validate our theoretical analysis in Sec. 5. In a synthetic setting where we have access to the Bayes classifier, our modified loss yields estimators that are closer to the Bayes classifier. Moreover, our enhanced distillation improve dramatically over vanilla distillation in failure regimes of the teacher,

e.g., when the teacher is heavily biased or overfitted. On five real tabular datasets, cross-fitting and corrected distillation improve the student's performance by up to 4% AUC point compared to vanilla KD. Furthermore, on a common image classification dataset (CIFAR-10, Krizhevsky & Hinton, 2009), when the teacher model overfits, cross-fitting and our corrected loss improve the student accuracy by up to 1.5%. This demonstrates the wide applicability of our enhancements.

Related work A number of papers have argued that the availability of soft class probabilities from the teacher rather than hard labels enables us to improve training of the student model. This was hypothesized in Hinton et al. (2015) with empirical justification. Phuong & Lampert (2019) consider the case where the teacher is a fixed linear classifier and the student is a linear classifier or a deep linear network. They show that the student can learn the teacher perfectly if it has access to training examples more than the ambient dimensions. Vapnik & Izmailov (2015) discusses the setting of learning with privileged information where one has additional information at training time which is not available at test time. Lopez-Paz et al. (2015) draws a connection between this and distillation, arguing that distillation is effective because the teacher learns a better representation allowing the student to learn at a faster rate. They hypothesize that a teacher's soft predictions indicating if an example is hard or easy enables this. Tang et al. (2020) argues using empirical evidence that label smoothing and reweighting of training examples using the teacher's predictions are key to benefits offered by knowledge distillation. Mobahi et al. (2020) analyzed the case of self-distillation where the student and teacher function classes are the same. They showed that this is equivalent to increasing regularisation strength for kernelized models. Bu et al. (2020) considers model compression in a rate-distortion framework, where the rate is the size of the student model and distortion is the difference in excess risk between the teacher and the student. Menon et al. (2020) consider the case of losses such that the population risk is linear in the Bayes class probabilities. They consider *distilled empirical risk* and *Bayes distilled empirical risk* which are the risk computed using the teacher class probabilities and Bayes class probabilities respectively rather than the observed label. They show that the variance of the Bayes distilled empirical risk is lower than the empirical risk. Then using analysis from Maurer & Pontil (2009); Bennett (1962), they derive the excess risk of the distilled empirical risk as a function of the ℓ_2 distance between the teacher's class probabilities and the Bayes class probabilities. We significantly depart from Menon et al. (2020) in multiple ways: i) our Thm. 1 allows for the common practice of data re-use, ii) our results cover the standard distillation losses (1) and (2) which are non-linear in p_0, iii) we use localized Rademacher analysis to achieve tight fast rates for strongly-convex losses; which the majority of distillation losses satisfies, iv) we use techniques from semiparametric inference to improve upon vanilla distillation.

2 Knowledge Distillation Background

In this section, we present our problem setup and an introduction to knowledge distillation. We are given a training dataset $\{(x_1,y_1),\ldots,(x_n,y_n)\}$ sampled independently from some probability distribution $\mathbb{P}$ with $w:=(x,y)\in\mathcal{X}\times\mathcal{Y}=:\mathcal{W}$. The goal is to learn some function $f\colon\mathcal{X}\to\mathcal{Y}$ from some function class $\mathcal{F}$ that minimizes the risk (i.e., expected loss over the population distribution $\mathbb{P}$):

$$L_D(f):=\mathbb{E}_{W\sim\mathbb{P}}[\ell(W;f(X))],$$

where $\ell\colon\mathcal{W}\times\mathcal{Y}\to\mathbb{R}$ is some given loss function. In multiclass classification with k classes, the label vector $y\in\{e_1,\ldots,e_j\}\subset\{0,1\}^k$ is a one-hot encoding of the class label.

Knowledge distillation Knowledge distillation (KD) is a two-step training process where one first uses a labeled dataset to train a teacher model and then trains a student model to predict the teacher's predicted class probabilities. Typically the teacher model is larger and more cumbersome, while the student is smaller and more efficient. Knowledge distillation was first motivated by model compression (Bucila et al., 2006), to find compact yet high-performing models to be deployed (such as on mobile devices).

In training the student to match the teacher's prediction probability, there are several types of loss functions that are commonly used. Let $\hat{p}(x)\in\mathbb{R}^k$ be the teacher's vector of predicted class probabilities, $f(x)\in\mathbb{R}^k$ be the student model's output, and $[k]\triangleq\{1,2,\ldots,k\}$. The most popular loss functions[1] $\ell(w;f(x),\hat{p}(x))$ include the squared error logit loss (Ba & Caruana, 2014)

$$\ell_{\text{se}}(w;f(x),\hat{p}(x))\triangleq\sum_{j\in[k]}\tfrac{1}{2}(f_j(x)-\log(\hat{p}_j(x)))^2 \tag{1}$$

[1]These loss functions do not depend on the label y, but we use the augmented notation $\ell(w;f(x),\hat{p}(x))$ to accommodate the enhanced distillation losses presented in Sec. 4.

and the annealed cross-entropy loss (Hinton et al., 2015)

$$\ell_\beta(w;f(x),\hat{p}(x)) = -\sum_{j\in[k]} \frac{\hat{p}_j(x)^\beta}{\sum_{l\in[k]}\hat{p}_l(x)^\beta} \log\left(\frac{\exp(\beta f_j(x))}{\sum_{l\in[k]}\exp(\beta f_l(x))}\right) \tag{2}$$

for an inverse temperature $\beta > 0$. These loss functions measure the divergence between the probabilities predicted by the teacher and the student.

A student model trained with knowledge distillation often performs better than the same model trained from scratch (Bucila et al., 2006; Hinton et al., 2015). In Secs. 3 and 4, we will adapt modern tools from semiparametric inference to understand and enhance this phenomenon.

3 Distillation as Semiparametric Inference

In semiparametric inference (Kosorok, 2007), one aims to estimate a target parameter or function f_0, but that estimation depends on an auxiliary *nuisance function* p_0 that is unknown and not of primary interest. We cast the knowledge distillation process as a semiparametric inference problem, by treating the teacher's probabilities as a nuisance function that approximates the Bayes probability $p_0(x) = \mathbb{E}[Y \mid X = x]$. This perspective allows us bound the generalization of the student in terms of the MSE between the teacher and the Bayes probabilities. In the next section (Sec. 4) we use techniques from semi-parametric inference to enhance the performance of the student.

Our analysis starts from taking the following perspective on distillation. We view the goal of the student as minimizing an oracle population loss over a function class $\mathcal{F}$,

$$L_D(f,p_0) = \mathbb{E}[\ell(W;f(X),p_0(X))] \quad \text{with} \quad f_0 \triangleq \operatorname{argmin}_{f\in\mathcal{F}} L_D(f,p_0).$$

The main hurdle is that this is objective depends on the unknown Bayes probabilities p_0. We view the teacher's model $\hat{p}$ as an approximate version of p_0 and bound the distillation error of the student as a function of the teacher's estimation error.

Typical semi-parametric inference considers cases where f_0 is a finite dimensional parameter, however recent work of Foster & Syrgkanis (2019) extends this framework to infinite dimensional models f_0 and proposes the statistical learning theory with a nuisance component framework. The distillation problem fits exactly into this setup.

Bounds on vanilla distillation with data re-use As a first step we derive a vanilla bound on the error of the distilled student model without any further modifications of the distillation process, i.e. we assume that the student is trained on the same data as the teacher and is trained by running empirical risk minimization on the plug-in loss, plugging in the teacher's model instead of p_0, i.e.,

$$\hat{f} = \operatorname{argmin}_{f\in\mathcal{F}} L_n(f,\hat{p}) \quad \text{for} \quad L_n(f,\hat{p}) \triangleq \mathbb{E}_n[\ell(W;f(X),\hat{p}(X))] \tag{3}$$

where $\mathbb{E}_n[X] = \frac{1}{n}\sum_{i=1}^n X_i$ denotes the empirical expectation of a random variable.

Technical definitions Before presenting our main theorem we introduce some technical notation. For a vector valued function f that takes as input a random variable X, we use the shorthand notation $\|f\|_{p,q} \triangleq \|\|f(X)\|_p\|_{L^q} = \mathbb{E}\left[\|f(X)\|_p^q\right]^{1/q}$. Let ∇_ϕ and ∇_π denote the partial derivatives of $\ell(w;\phi,\pi)$, with respect to its second and third input correspondingly and $\nabla_{\phi\pi}$ the Jacobian of cross partial derivatives, i.e. $[\nabla_{\phi\pi}\ell(w;\phi,\pi)]_{i,j} = \frac{\partial^2}{\partial\phi_j\partial\pi_i}\ell(w;\phi,\pi)$. Finally, let $q_{f,p}(x) = \mathbb{E}[\nabla_{\phi\pi}\ell(W;f(X),p(X)) \mid X = x]$ and $\gamma_{f,p}(x) = \mathbb{E}_{U\sim\text{Unif}([0,1])}[q_{f,Up+(1-U)p_0}(x)]$.

Critical radius Finally, we need to define the notion of the critical radius (see e.g., Wainwright (2019)) of a function class, which typically provides tight learning rates for statistical learning theory tasks. For any function class $\mathcal{F}$ we define the localized Rademacher complexity as:

$$\mathcal{R}(\delta;\mathcal{F}) = \mathbb{E}_{X_{1:n},\epsilon_{1:n}}[\sup_{f\in\mathcal{F}:\|f\|_2\le\delta} \tfrac{1}{n}\textstyle\sum_{i=1}^n \epsilon_i f(X_i)]$$

where ϵ_i are i.i.d. random variables taking values equiprobably in $\{-1,1\}$. The *critical radius* of a class $\mathcal{F}$, taking values in $[-H,H]$, is the smallest solution δ_n to the inequality $\mathcal{R}(\delta;\mathcal{F}) \le \frac{\delta^2}{H}$.

Theorem 1 (Vanilla distillation)**.** *Assume that $f_0 \in \mathcal{F}$ and $\mathcal{F}$ is a convex set and that the teacher estimates a model $\hat{p} \in \mathcal{P}$ on the same sample as the student. Let $\delta_{n,\zeta} = \delta_n + c_0\sqrt{\frac{\log(c_1/\zeta)}{n}}$ for some universal constants c_0, c_1 and δ_n is an upper bound on the critical radius the function class:*

$$\mathcal{G} \triangleq \{w \to r(\ell(w;f(x),p(x)) - \ell(w;f_0(x),p(x))) : f\in\mathcal{F}, p\in\mathcal{P}, r\in[0,1]\}$$

Assume that, for all $w \in \mathcal{W}$ and π, the loss $\ell(w;\phi,\pi)$ is σ-strongly convex with respect to ϕ, uniformly bounded in $[-H,H]$ for all w,ϕ,π and let: $\mu(w) = \sup_\phi \|\nabla_\phi \ell(w;\phi,\hat{p}(x))\|_2$. Moreover, suppose that

the function class f satisfies the ℓ_2/ℓ_4 ratio condition: $\sup_{f\in\mathcal{F}}\frac{\|f-f_0\|_{2,4}}{\|f-f_0\|_{2,2}}\leq C$. *Then* $\hat{f}$ (3) *satisfies*

$$\|\hat{f}-f_0\|_{2,2}^2\leq\frac{1}{\sigma^2}O(\delta_{n,\zeta}^2C^2H^2\|\mu\|_4^2+\|\gamma_{f_0,\hat{p}}^\top(\hat{p}-p_0)\|_{2,2}^2)\quad\textit{with probability}\quad 1-\zeta.$$

Remark The proof is in App. B. We note that the ℓ_2/ℓ_4 ratio requirement can be removed, albeit the final bound will depend on a uniform bound $\|\mu\|_\infty=\sup_w|\mu(w)|$, instead of $\|\mu\|_4$. Moreover, we note that the strong convexity requirement for ℓ is satisfied by all standard distillation objectives, as it is strong convexity with respect to the output of f and not the parameters of f. Even this requirement could be removed, but this would yield slow rate bounds of the form: $\|\hat{f}-f_0\|_{2,2}^2=O(\delta_{n,\zeta}+\|\gamma_{f_0,\hat{p}}^\top(\hat{p}-p_0)\|_{2,2}^2)$.

Thm. 1 shows that the standard approach to distillation can provably work to provide an accurate student and potentially improve upon training from scratch. For instance, if the teacher is very accurate, i.e. $\hat{p}\approx p_0$, then the term that remains contains the fourth moment of the loss gradient $\|\mu\|_4$. If we were to replace the student $\hat{p}(x)$, with the raw labels y, then we would have gotten a dependence on the fourth moment of the loss gradient $\tilde{\mu}(w)\triangleq\sup_{f\in\mathcal{F}}\|\nabla_\phi\ell(w;f(x),y)\|_2$, which now contains extra variation due to the variance of the labels y. Thus in practice it can be that $\|\mu\|_4\ll\|\tilde{\mu}\|_4$.

Drawbacks of vanilla distillation There are two major drawbacks of Thm. 1, which are inherent drawbacks of vanilla distillation. First, the function class $\mathcal{G}$ contains the variation of the student's model over the whole $\mathcal{P}$. If $\mathcal{P}$ is a large model space, with a large critical radius, then $\mathcal{G}$, will inherit this complexity and the final bound will depend on the sample complexity of the teacher. Second, if the teacher is not very accurate, i.e. $\|\hat{p}-p_0\|_{2,2}$ is large, then the student's model will be significantly impacted. In the next section, we use techniques from semi-parametric inference to tackle both of these problems.

4 Enhancing Knowledge Distillation

We can view the plug-in distillation loss $\ell(w;f(x),\hat{p}(x))$ as a zeroth order Taylor approximation to the ideal loss $\ell(w;f(x),p_0(x))$ around $\hat{p}$. An ideal first-order Taylor approximation to the loss would take the form

$$\ell(w;f(x),\hat{p}(x))+\langle p_0(x)-\hat{p}(x),\nabla_\pi\ell(w;f(x),\hat{p}(x))\rangle.$$

However, its computation also requires knowledge of p_0. Nevertheless, since $p_0(x)=\mathbb{E}[Y\mid X=x]$, we can always construct an unbiased estimate of the ideal first order term by replacing $p_0(x)$ with y:

$$\ell_{ortho}(w;f(x),\hat{p}(x))=\ell(w;f(x),\hat{p}(x))+\langle y-\hat{p}(x),\mathbb{E}[\nabla_\pi\ell(w;f(x),\hat{p}(x))\mid x]\rangle$$

This correction in the direction of $y-\hat{p}$ can potentially improve approximation error. To allow more flexibility so as to balance bias and variance, we consider a more general form of a correction term, which we call the γ-*corrected loss* for $\gamma:\mathcal{X}\to\mathbb{R}^k\times\mathbb{R}^k$ a matrix valued function:

$$\ell_\gamma(w;f(x),p(x))\triangleq\ell(w;f(x),p(x))+(y-p(x))^\top\gamma(x)f(x).$$

We denote associated population and empirical risks by

$$L_D(f,p,\gamma)\triangleq\mathbb{E}[\ell_\gamma(W;f(X),p(X))]\quad\text{and}\quad L_n(f,p,\gamma)\triangleq\mathbb{E}_n[\ell_\gamma(W;f(X),p(X))].$$

Observe that at p_0 the correction term is mean-zero and hence $L_D(f,p_0,\gamma)$ is independent of γ

$$L_D(f,p_0)\triangleq\mathbb{E}[\ell(W;f(X),p_0(X))]=L_D(f,p_0,\gamma)\quad\text{for all}\quad\gamma.$$

4.1 Robustness of γ-Corrected Loss to Teacher Error

The γ-corrected loss has strong connections to the literature on Neyman orthogonality (Chernozhukov et al., 2018; Chernozhukov et al., 2016; Nekipelov et al., 2018; Chernozhukov et al., 2018; Foster & Syrgkanis, 2019). In particular, if the function γ is set appropriately, then one can show that the γ-corrected loss function satisfies the condition of a Neyman orthogonal loss defined by Foster & Syrgkanis (2019). We begin our analysis by showing a general lemma for any estimator $\hat{f}$, which adapts the main theorem of Foster & Syrgkanis (2019) to account for approximate orthogonality; the proof can be found in App. A.

Lemma 2 (Algorithm-agnostic analysis)**.** *Consider any estimation algorithm that produces an estimate $\hat{f}$ with small plug-in excess risk, i.e.,*

$$L_D(\hat{f},\hat{p},\gamma)-L_D(f_0,\hat{p},\gamma)\leq\epsilon(\hat{f},\hat{p},\gamma)$$

and that the loss L_D is σ-strongly convex with respect to f and $\mathcal{F}$ is a convex set. Then:

$$\tfrac{\sigma}{4}\|\hat{f}-f_0\|_{2,2}^2\leq\epsilon(\hat{f},\hat{p},\gamma)+\tfrac{1}{\sigma}\|(\gamma_{f_0,\hat{p}}-\gamma)^\top(\hat{p}-p_0)\|_{2,2}^2$$

If, further, $\sup_{w,\phi,\pi,i\in[d]}\|\nabla_{\phi_i\pi\pi}\ell(w;\phi,\pi)\|_{\text{op}}\leq M$, *then:*

$$\|(\gamma_{f_0,\hat{p}}-\gamma)^\top(\hat{p}-p_0)\|_{2,2}^2\leq2\big(\|(q_{f_0,\hat{p}}-\gamma)^\top(\hat{p}-p_0)\|_{2,2}^2+M^2k\|\hat{p}-p_0\|_{2,4}^4\big)$$

Connection to Neyman orthogonality Note that if we set $\gamma = q_{f_0,\hat{p}}$, then we obtain that the MSE error of the student depends on the MSE error of the teacher only in a second order manner! Morever, as we show in the Example 3, $q_{f_0,\hat{p}}$ is typically independent of f and hence a known closed form function of $\hat{p}$. Setting $\gamma = q_{f_0,\hat{p}}$ renders the loss function Neyman orthogonal (Foster & Syrgkanis, 2019). However, we note that this setting of the γ can lead to larger variance, i.e., the achievable excess risk can be much larger than the excess risk without the γ-correction. For instance, in the case of the squared error logit loss $q_{f_0,\hat{p}}(x) = \frac{1}{\hat{p}(x)}$, which can be really large when $\hat{p}$ is close to 0, leading to a large increase in the variance of our loss. Thus unlike the standard approach in semiparametric inference, we will be choosing γ in practice to balance bias and variance.

Example 3 (Bregman Divergence Losses)**.** *For any* Bregman divergence *loss function of the form*

$$\ell(w;\phi,\pi) \triangleq \Psi(\phi) - \Psi(g(\pi)) - \langle \nabla\Psi(g(\pi)), \phi - g(\pi)\rangle \quad \textit{we have}$$

$$\ell_\gamma(w;\phi,\pi) = \Psi(\phi) - \langle \nabla\Psi(g(\pi)) + \gamma(x)^\top(y-\pi), \phi\rangle + \text{const}.$$

For such losses, the quantities $q_{f,p}$ and $\gamma_{f,p}$ are independent of f, since:

$$\forall f,p : q_{f,p}(x) = \mathbb{E}[\nabla_{\phi\pi}\ell(W;f(X),p(X)) \,|\, X=x] = \nabla g(p(x))^\top \nabla^2\Psi(g(p(x))) =: q_p(x)$$

Thus by choosing $\gamma = q_{\hat{p}}$, which is a known closed form function of the teacher's model, we achieve a second order dependence on the teacher's estimation error. For the squared error logit loss (1)*, $\Psi(s) = \frac{1}{2}\|s\|_2^2$, $g(p) = \log(p)$, and $q_p(x) = \text{diag}\left(\frac{1}{p_1(x)},\ldots,\frac{1}{p_K(x)}\right)$. Similarly, the* annealed cross-entropy loss (2) *falls into the class of Bregman divergence losses.*

Example instantiation of student's estimation algorithm If we use *plug-in empirical risk minimization*, i.e., $\hat{f} = \text{argmin}_{f\in\mathcal{F}} L_n(f,\hat{p},\gamma)$, to estimate f_0 with $\hat{p}$ estimated on an independent sample, then the results of Maurer & Pontil (2009) directly imply that as long as the loss function $\ell(w;\phi,\pi)$ is uniformly bounded in $[-H,H]$, then w.p. $1-\delta$:

$$\epsilon(\hat{f},\hat{p},\gamma) \leq O\Big(\sqrt{\frac{\sup_{f\in\mathcal{F}}\text{Var}(\ell_\gamma(W;f(X),\hat{p}(X)))\log(\tau(n)/\delta)}{n}} + \frac{H\log(\tau(n)/\delta)}{n}\Big)$$

where $\tau(n) = \mathcal{N}_\infty(1/n,\mathcal{F},2n)$ and $\mathcal{N}_\infty(\epsilon,\mathcal{F},m)$ is the ℓ_∞ empirical covering number of function class $\mathcal{F}$ in the worst-case over all realizations of m samples and at approximation level ϵ. This result has two drawbacks: it is a slow rate result that scales as $1/\sqrt{n}$ for parametric of bounded VC-dimension classes and it requires the student to be fit on a completely separate sample than the teacher. In the next theorem, we address both of these drawbacks: i) we invoke localized Rademacher complexity analysis to provide a fast rate result which would be of the order of $1/n$ for VC or parametric function classes, ii) we use a more sophisticated sample-splitting technique called cross-fitting, which allows the student to be trained on all the available data.

4.2 Cross-fitted ERM analysis

We now provide a more sophisticated version of sample splitting to make use of all datapoints in our final estimation, while at the same time not taking a hit by the sample complexity of the teacher's function space. This approach is referred to as *cross-fitting* in the semiparametric inference literature (see e.g., Chernozhukov et al. (2018)):

1. Partition the dataset into B equally sized partitions $P_1,\ldots,P_B$
2. For each fold $t \in [B]$ estimate $\hat{p}^{(t)}$ and $\hat{\gamma}^{(t)}$ using all the out-of-fold samples
3. Estimate $\hat{f}$ by minimizing the empirical loss:

$$\hat{f} = \text{argmin}_{f\in\mathcal{F}} \frac{1}{n}\sum_{t=1}^{B}\sum_{i\in P_t} \ell_{\hat{\gamma}^{(t)}}(W_i;f(X_i),\hat{p}^{(t)}(X_i))$$

In other words, the nuisance estimates $\hat{\gamma}^{(t)},\hat{p}^{(t)}$ that are evaluated on the samples in fold t, are estimated based only on samples outside of P_t.

Theorem 4 (Cross-fitted ERM analysis)**.** *Assume that $f_0 \in \mathcal{F}$ and $\mathcal{F}$ is a convex set. Let $\delta_{n,\zeta} = \delta_n + c_0\sqrt{\frac{\log(c_1/\zeta)}{n}}$ for some universal constants c_0,c_1 and δ_n is an upper bound on the critical radii of the classes:*

$$\mathcal{G}(\hat{p}^{(t)},\hat{\gamma}^{(t)}) = \{w \to r\big(\ell_{\hat{\gamma}^{(t)}}(w;f(x),\hat{p}^{(t)}(x)) - \ell_{\hat{\gamma}^{(t)}}(w;f_0(x),\hat{p}^{(t)}(x))\big) : f\in\mathcal{F}, r\in[0,1]\}$$

for each $t \in [B]$. Assume that, for all $w \in \mathcal{W}$ and π, the loss $\ell(w;\,\phi,\,\pi)$ is σ-strongly convex with respect to ϕ, uniformly bounded in $[-H,\,H]$ for all w, ϕ, π and let: $\mu(w) = \sup_{f\in\mathcal{F},t\in[B]}\big\|\nabla_\phi\ell(w;f(X),\hat{p}^{(t)}(x))\big\|_2$. Moreover, suppose that the function class f satisfies the ℓ_2/ℓ_4 ratio condition: $\sup_{f\in\mathcal{F}}\frac{\|f-f_0\|_{2,4}}{\|f-f_0\|_{2,2}} \leq C$. If $\hat{f}$ is the output of the cross-fitted empirical risk

minimization algorithm on a fresh set of n samples, then, w.p. $1-\zeta$:

$$\frac{\sigma}{8}\|\hat{f}-f_0\|_{2,2}^2 \leq \frac{1}{\sigma}O\Big(\delta_{n/B,\zeta/B}^2 C^2 H^2\Big(\|\mu\|_4^2+\frac{1}{B}\sum_{t=1}^B\sqrt{\mathbb{E}\big[\|(Y-\hat{p}^{(t)}(X))^\top\hat{\gamma}^{(t)}(X)\|_2^4\big]}\Big)\Big)$$
$$+\frac{1}{\sigma}O\big(\frac{1}{B}\sum_{t=1}^B\|(\gamma_{f_0,\hat{p}^{(t)}}-\hat{\gamma}^{(t)})^\top(\hat{p}^{(t)}-p_0)\|_{2,2}^2\big).$$

The proof is found in App. C. Observe that unlike Thm. 1, the function classes $\mathcal{G}(\hat{p}^{(t)},\hat{\gamma}^{(t)})$ in the latter theorem do not vary the teacher's model over $\mathcal{P}$, but rather only vary $f\in\mathcal{F}$ and evaluate p at the out-of-fold estimate $p^{(t)}$. Since in practice the teacher's model can be quite complex, getting rid of this dependence on the sample complexity of the teacher's function space can bring immense improvement. Thus the critical radius of $\mathcal{G}(\hat{p}^{(t)},\hat{\gamma}^{(t)})$, can be significantly smaller than $\mathcal{G}$. For instance, if $\mathcal{P}$ and $\mathcal{F}$ are VC-subgraph classes with VC dimensions $d_{\mathcal{P}}\gg d_{\mathcal{F}}$, correspondingly, then the critical radius of $\mathcal{G}(\hat{p}^{(t)},\hat{\gamma}^{(t)})$, will be of the order $\sqrt{d_{\mathcal{F}}\log(n)/n}$, while that of $\mathcal{G}$ of the order of $\sqrt{d_{\mathcal{P}}\log(n)/n}$.

Moreover, we can see in the bound of Thm. 4 the interplay between bias and variance introduced by γ. In particular, the part of the bound that depends on γ can be further simplified as:

$$\sqrt{\mathbb{E}[\delta_{n,\zeta}^4 C^4\|(Y-\hat{p}(X))^\top\gamma(X)\|_2^4+\|(\gamma_{\hat{p},0}(X)-\gamma(X))^\top(\hat{p}(X)-p_0(X))\|_2^4]}$$

where the first part corresponds to the bias increase due to γ, while the second part the bias decrease.

4.3 Biased stochastic gradient descent analysis

When the set of candidate prediction rules f_θ is parameterized by a vector $\theta\in\mathbb{R}^d$, we may alternatively fit θ via stochastic gradient descent (SGD) (Robbins & Monro, 1951; Bottou & Bousquet, 2008) on the γ-corrected objective $L_D(f_\theta,\hat{p},\gamma)$. With a minibatch size of 1 and a starting point θ_0, the parameter updates take the form

$$\theta_{t+1}=\theta_t-\eta_t\nabla_\theta f_\theta(X_t)^\top\nabla_\phi\ell_\gamma(W_t;f_\theta(X_t),p(X_t)) \quad \text{for} \quad t+1\in[n]. \tag{4}$$

Ideally, these updates would converge to a minimizer of the ideal risk $\mathcal{L}(\theta;p_0)=L_D(f_\theta,p_0)$. Our next result shows that, if the teacher $\hat{p}$ is independent of $(W_t)_{t\in[n]}$, then the SGD updates (4) have excess ideal risk governed by a bias term $\zeta(\gamma)$ and a variance term $\sigma(\gamma)^2/n$. Here, $\sigma_0^2(\theta)$ represents the baseline stochastic gradient variance that would be incurred if SGD were run directly on the ideal risk $\mathcal{L}(\theta;p_0)$ rather than our surrogate risk. Our proof in App. D builds upon the biased SGD bounds of Ajalloeian & Stich (2020).

Theorem 5 (Biased SGD analysis)**.** *Suppose that the loss $\mathcal{L}(\theta;p_0)$ is λ-strongly smooth in θ. Define the bias and root-variance parameters*

$$\zeta(\gamma)\triangleq\sup_{\theta\in\mathbb{R}^d}\big\|\nabla_\theta f_\theta^\top(\gamma_{f_\theta,\hat{p}}-\gamma)^\top(\hat{p}-p_0)\big\|_{2,2}$$

$$\sigma(\gamma)\triangleq\sup_{\theta\in\mathbb{R}^d}\sigma_0(\theta)+\sqrt{\mathbb{E}[\|\nabla_\theta f_\theta(X)^\top\gamma(X)^\top(Y-p_0(X))\|_2^2]+\big\|\nabla_\theta f_\theta^\top(\gamma_{f_\theta,\hat{p}}-\gamma)^\top(\hat{p}-p_0)\big\|_{2,2}^2}$$

for $\sigma_0^2(\theta)\triangleq\sum_{i\in[d]}\mathrm{Var}[\nabla_{\theta_i}\ell(W;\ f_\theta(X),\ p_0(X))]$ the unbiased SGD variance. If $F_0=\mathcal{L}(\theta_0;p_0)-\min_{\theta\in\mathbb{R}^d}\mathcal{L}(\theta;p_0)$, then the iterates $\{\theta_t\}_{t=1}^n$ of the γ-corrected SGD algorithm satisfy

$$\min_{t\in[n]}\mathbb{E}\big[\|\nabla_\theta\mathcal{L}(\theta_t;p_0)\|_2^2\big]=O\Big(\frac{\sigma(\gamma)\sqrt{\lambda F_0}}{\sqrt{n}}+\zeta^2(\gamma)\Big).$$

If, in addition, $\mathcal{L}(\theta;p_0)$ is μ-strongly convex in θ, then the iterates satisfy

$$\mathbb{E}[\mathcal{L}(\theta_n;p_0)-\min_{\theta\in\mathbb{R}^d}\mathcal{L}(\theta;p_0)]=\frac{1}{\mu}O\Big(\frac{\lambda}{\mu}\frac{\sigma(\gamma)^2}{n}+\zeta^2(\gamma)\Big)+O\big(F_0e^{-\frac{\mu}{2\lambda}n}\big).$$

Similar to Thm. 4, the bound in Thm. 5, portrays the interplay of bias and variance as γ ranges from 0 to $q_{f_\theta,\hat{p}}$ (which we remind that for any Bregman loss is independent of f_θ). In particular, the part of the bound for strongly convex losses that depends on γ can be further simplified to:

$$\mathbb{E}\Big[\Big(\frac{\lambda\|\gamma(X)\|_2^2\|Y-p_0(X)\|_2^2}{\mu n}+\|(\gamma_{f_\theta,\hat{p}}(X)-\gamma(X))^\top(\hat{p}(X)-p_0(X))\|_2^2\Big)\|\nabla_\theta f_{\hat{\theta}}(X)\|_2^2\Big]$$

This has a very intuitive form: the first term is the impact of $\gamma(X)$ on the variance, which is also related to the square of the noise of y, divided by the standard error scaling. The second controls how γ improves the bias introduced by the error in the teacher's $\hat{p}$. Both the variance and the bias are re-weighted based on the gradient of θ, which expresses that some regions of X are more important in identifying the parameters and therefore, when we minimize the average bias-variane trade-off, we should be re-weighting the samples based on how informative they are about the parameters θ.

5 EXPERIMENTS

We empirically validate that the two components of our solution, cross-fitting and corrected loss function, can improve the student's performance, in a variety of settings: (i) a synthetic setting that validates the theory in Secs. 3 and 4, (ii) tabular data showing that cross-fitting and γ-correction yield improvement, and (iii) image data to show the wide applicability of our methods. Throughout, we use the squared error logit loss (1). Additional experiment details and results are described in App. E.

Objective for picking γ in correction. Motivated by the analysis in Secs. 4.1 and 4.3, we propose to find the correction γ by balancing the bias and variance terms. In particular, at each point (x,y), we choose $\gamma(x) = \mathrm{diag}(v(x))$ to minimize

$$\|v(x)\|_2^2 \mathbb{E}[\|y-\hat{p}(x)\|_2^2 \,|\, x] + \alpha \|q_{\hat{p}}(x) - v(x)\|_2^2,$$

where the hyperparameter α controls the exact tradeoff between bias and variance. Since the conditional expectation involves the unknown quantity p_0, we approximate $\mathbb{E}[\|y-\hat{p}(x)\|_2^2 \,|\, x]$ by its sample $\|y-\hat{p}(x)\|_2^2$.[2] These two terms are simplified versions of the terms in Thm. 5. Note that this objective is a quadratic function in $v(x)$, and thus has closed-form solution that is fast to compute. In the case of squared error logit-loss, $q_{\hat{p}}(x) = 1/\hat{p}(x)$ and in the case of squared loss $q_{\hat{p}}(x) = 1$. Moreover, once we solve for $\gamma(x)$, the student's γ-corrected objective can be shown to be equivalent to a square loss with labels equal to $\log(p(x)) + \gamma(x)^\top (y - p(x))$.

Validation of theoretical analysis When the Bayes probability $p_0(x)$ is known, we validate that the corrected loss function yields a student model whose accuracy is closer to the performance of the Bayes classifier, compared to a student model trained from scratch.

The synthetic data is generated from a mixture of two Gaussians with equal weights, where the Bayes classifier is known. The student model is a linear logistic regression model, which can capture the Bayes classifier. To simulate the teacher probabilities, we take the true probability $p_0(x)$ and move it closer to either 0 or 1, whichever is closer to $p_0(x)$. We compare 4 training objectives for the student model: (i) trained from scratch (ii) trained with vanilla KD (iii) trained with γ-corrected KD loss (iv) trained to match the Bayes probability $p_0(x)$. Figure 1 shows that the corrected KD loss brings the student's accuracy close to the case where it is trained on the true probabilities.

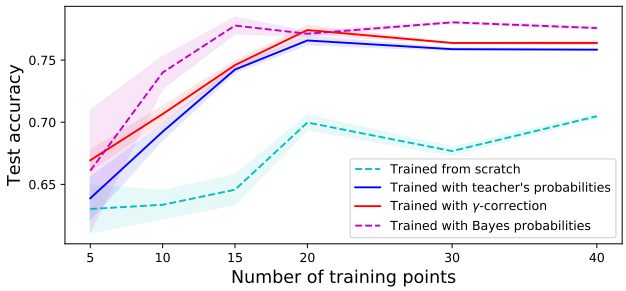


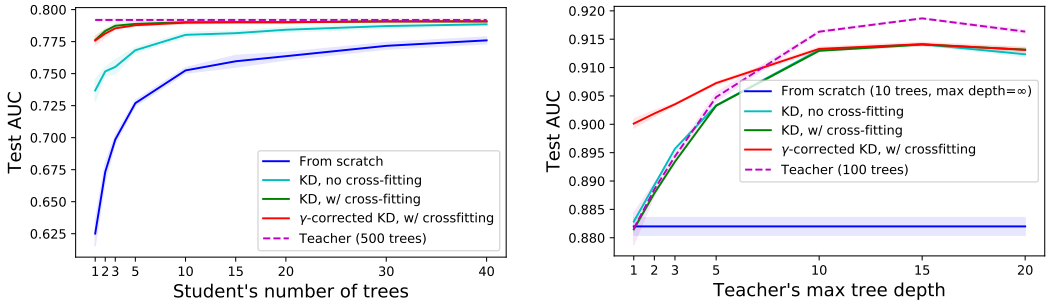
Figure 1: On synthetic dataset, γ-correction helps de-bias the teacher, bringing student's accuracy closer to when trained on true p_0.

Tabular data We validate cross-fitting and corrected KD loss on five real-world tabular datasets datasets: Adult (Dheeru & Karra Taniskidou, 2017), FICO (FIC), Higgs (Dheeru & Karra Taniskidou, 2017), MAGIC (Dheeru & Karra Taniskidou, 2017), and StumbleUpon (Eve; Liu et al., 2017). Cross-fitting can improve the student performance by up to 0.04 AUC points when the teacher model likely overfits, while γ-corrected KD loss is most helpful when the teacher has high bias.

We validate that cross-fitting can improve KD when the teacher overfits, and γ-correction is helpful when the teacher has high bias. Both teacher and student models are random forest. In the first case (Fig. 2a), we use a large teacher (500 trees) and vary the student's capacity, while in the second case (Fig. 2b) we vary the teacher's bias by limiting the teacher's max tree depth. Figure 2 shows the result of the first case on the FICO dataset, and the results of the second case on the Adult dataset. The results on the rest of the datasets are similar (App. E.2). When the teacher overfits, cross-fitting shows significant improvement over using the same teacher on the training points. The γ correction

[2] An alternative that performs slightly worse is to approximate $\mathbb{E}[\|y-\hat{p}(x)\|^2 \,|\, x]$ by $\|\hat{p}(x)(1-\hat{p}(x))\|_2^2$.

successfully reduces the teacher's bias and thus improves the student's performance. The effect is most pronounced when the teacher has large bias (low tree depth).



(a) FICO dataset, when teacher overfits

(b) Adult dataset, when teacher has high bias

Figure 2: Cross-fitting leads to better KD when the teacher overfits, while γ-correction improves student's performance when the teacher has high bias.

Image data On the image classification dataset CIFAR-10 (Krizhevsky & Hinton, 2009), we show that cross-fitting can improve the student's performance in the case where the teacher overfits. We use ResNet-8 as the student and ResNet-14/20/32/44/56 (He et al., 2016) as the teacher. It has been observed that larger or deeper teachers might not yield better students, as the teacher might overfit to the training set (Cho & Hariharan, 2019; Müller et al., 2019). To simulate overfitting, we turn off data augmentation (random horizontal flipping and cropping). We compare students trained with vanilla KD objective with and without cross-fitting and γ-correction in Fig. 3. Cross-fitting can reduce the effect of teacher's overfitting, especially for deep teacher models. This effect is most evident in the test loss, where the student that is trained with vanilla KD has much higher loss than the student trained with KD and cross-fitting. The γ-correction consistently provides a small performance boost.

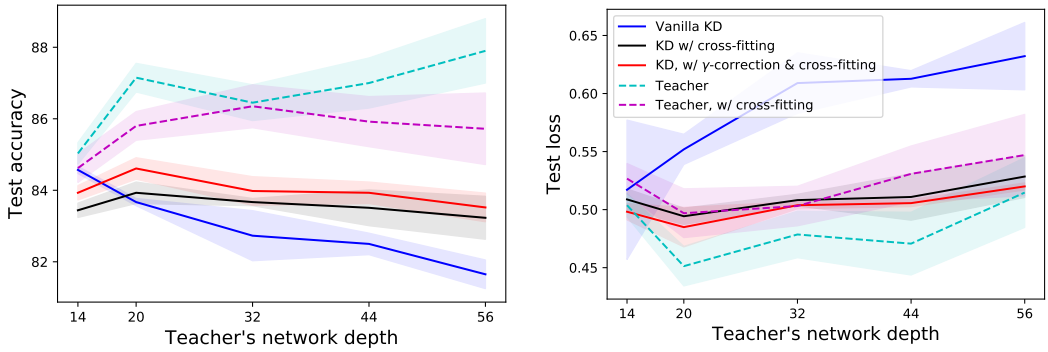


Figure 3: On CIFAR-10, cross-fitting reduces the effect of overfitting teacher, and γ-correction yields an additional small performance boost.

6 Conclusion

We provide a new analysis of knowledge distillation under the lens of semiparametric inference. By viewing the KD process as learning a student model with the true class probabilities as a nuisance function and the teacher's probabilities as a plug-in estimator, we obtain generalization bounds on the student model. This perspective also suggests two techniques to improve KD, namely cross-fitting and γ-correction, which we show leads to better KD performance, both theoretically and empirically. This also opens the door to combining KD with other techniques and corrections in the semiparametric literature, such as those based on targeted maximum likelihood framework (Van Der Laan & Rubin, 2006). We are excited about future work on unraveling many surprising phenomena in KD, such as the success of self-distillation (Furlanello et al., 2018) and noisy student training (Xie et al., 2020).

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A Proof of Lemma 2: Algorithm-agnostic analysis

First we define for any functional $L(f)$ the Frechet derivative as:

$$D_f L(f)[\nu] = \frac{\partial}{\partial t} L(f+t\nu)\,|_{t=0}$$

When L is an operator of the form: $\mathbb{E}[g(f(X))]$, then: $D_f L(f)[\nu] = \mathbb{E}[\nabla g(f(X))^\top \nu(X)]$.

By σ-strong convexity of L_D,[3] we have that

$$L_D(\hat{f},\hat{p},\gamma) \geq L_D(f_0,\hat{p},\gamma) + D_f L_D(f_0,\hat{p},\gamma)[\hat{f}-f_0] + \frac{\sigma}{2}\|\hat{f}-f_0\|_{2,2}^2.$$

Furthermore, our excess risk assumption and the optimality of f_0 give us

$$\begin{aligned}\frac{\sigma}{2}\|\hat{f}-f_0\|_{2,2}^2 &\leq \underbrace{L_D(\hat{f},\hat{p},\gamma) - L_D(f_0,\hat{p},\gamma)}_{\text{excess risk of } \hat{f}} - D_f L_D(f_0,\hat{p},\gamma)[\hat{f}-f_0] \\ &\overset{(a)}{\leq} \epsilon(\hat{f},\hat{p},\gamma) - \underbrace{D_f L_D(f_0,p_0,\gamma)[\hat{f}-f_0]}_{\geq 0 \text{ by optimality of } f_0} + D_f(L_D(f_0,p_0,\gamma) - L_D(f_0,\hat{p},\gamma))[\hat{f}-f_0].\end{aligned}$$

By Taylor's theorem with integral remainder,

$$\begin{aligned}&\mathbb{E}[\langle \nabla_\phi \ell(W;f_0(x),p_0(x)) - \nabla_\phi \ell(W;f_0(x),\hat{p}(x)), \hat{f}(x)-f_0(x)\rangle \,|\, X=x] \\ &= (p_0(x)-\hat{p}(x))^\top \gamma_{f_0,\hat{p}}(x)(\hat{f}(x)-f_0(x))\end{aligned} \tag{5}$$

whenever $\nabla_{\phi\pi}\ell$ is well-defined. We can now invoke the expansion (5) and Cauchy-Schwarz to obtain the bound

$$\begin{aligned}&D_f(L_D(f_0,p_0,\gamma) - L_D(f_0,\hat{p},\gamma))[\hat{f}-f_0] \\ &= \mathbb{E}[\langle \nabla_\phi \ell(W;f_0(X),p_0(X)) - \nabla_\phi \ell(W;f_0(X),p(X)), \hat{f}(X)-f_0(X)\rangle] \\ &\quad - \mathbb{E}[(p_0(X)-\hat{p}(X))^\top \gamma(X)(\hat{f}(X)-f_0(X))] \\ &= \mathbb{E}[(p_0(X)-\hat{p}(X))^\top (\gamma_{f_0,\hat{p}}(X)-\gamma(X))(\hat{f}(X)-f_0(X))] \\ &\leq \mathbb{E}[\|(p_0(X)-\hat{p}(X))^\top (\gamma_{f_0,\hat{p}}(X)-\gamma(X))\|_2 \|\hat{f}(X)-f_0(X)\|_2] \\ &\leq \|(p_0-\hat{p})^\top(\gamma_{f_0,\hat{p}}-\gamma)\|_{2,2}\|\hat{f}-f_0\|_{2,2}\end{aligned}$$

Thus combining all the above inequalities:

$$\frac{\sigma}{2}\|\hat{f}-f_0\|_{2,2}^2 \leq \epsilon(\hat{f},\hat{p},\gamma) + \|(\hat{p}-p_0)^\top(\gamma_{f_0,\hat{p}}-\gamma)\|_{2,2}\|\hat{f}-f_0\|_{2,2}$$

By an AM-GM inequality, for all $a,b \geq 0$: $a\cdot b \leq \frac{1}{2}(\frac{2}{\sigma}a^2 + \frac{\sigma}{2}b^2)$. Applying this to the product of norms on the RHS and re-arranging yields

$$\frac{\sigma}{4}\|\hat{f}-f_0\|_{2,2}^2 \leq \epsilon(\hat{f},\hat{p},\gamma) + \frac{1}{\sigma}\|(\hat{p}-p_0)^\top(\gamma_{f_0,\hat{p}}-\gamma)\|_{2,2}^2.$$

To get the final ineguality, observe that:

$$\|(\hat{p}-p_0)^\top(\gamma_{f_0,\hat{p}}-\gamma)\|_{2,2}^2 \leq 2\|(\hat{p}-p_0)^\top(q_{f_0,\hat{p}}-\gamma)\|_{2,2}^2 + 2\|(\hat{p}-p_0)^\top(\gamma_{f_0,\hat{p}}-q_{f_0,\hat{p}})\|_{2,2}^2$$

Moreover, by the boundedness of the third derivative, we have:

$$\begin{aligned}\|(\hat{p}-p_0)^\top(\gamma_{f_0,\hat{p}}-q_{f_0,\hat{p}})\|_{2,2}^2 &\leq \mathbb{E}[\|\hat{p}(X)-p_0(X)\|_2^2 \|\gamma_{f_0,\hat{p}}(X)-q_{f_0,\hat{p}}(X)\|_2^2] \\ &\leq \mathbb{E}[\|\hat{p}(X)-p_0(X)\|_2^2 M^2 k \|\hat{p}(X)-p_0(X)\|_2^2] \\ &\leq M^2 k \|\hat{p}-p_0\|_{2,4}^4\end{aligned}$$

Combining all the above yields the final bound.

B Proof of Theorem 1

Proof First by localized Rademacher analysis (see Lemma 11 of Foster & Syrgkanis (2019)) if δ_n upper bounds the critical radius of the function class $\mathcal{G}$ and if we denote with $\ell_{\hat{p},f}(w) = \ell(w;f(x),\hat{p}(x))$, then w.p. $1-\zeta$:[4]

$$\left|L_n(\hat{f},\hat{p}) - L_n(f_0,\hat{p}) - (L_D(\hat{f},\hat{p}) - L_D(f_0,\hat{p}))\right| \leq O\left(\delta_{n,\zeta}\|\ell_{\hat{p},\hat{f}} - \ell_{\hat{p},f_0}\|_{2,2} + \delta_{n,\zeta}^2\right)$$

[3] Notably this strong convexity assumption can be relaxed to $\mathbb{E}\left[\nabla_\phi \ell(W;f_0(X),p_0(X))(\hat{f}(X)-f_0(X)\right] \geq 0$.

[4] We apply the lemma with $\mathcal{L}_g = g$ and $g \in \mathcal{G}$ and $g^* = 0$. Then we instantiate the concentration inequality with $g = \ell_{\hat{p},\hat{f}} - \ell_{\hat{p},f_0} \in \mathcal{G}$.

Moreover, if we let $\mu(w) = \sup_\phi \|\nabla_\phi \ell(w;\phi,\hat{p}(x))\|_2$, then we have by Cauchy-Scwarz inequality:

$$\|\ell_{\hat{p},f} - \ell_{\hat{p},f_0}\|_{2,2} \leq \|\mu\|_4 \|f - f_0\|_{2,4}$$

If we further assume that the function class $\mathcal{F}$ satisfies an ℓ_2/ℓ_4 condition that:

$$\sup_{f\in\mathcal{F}} \frac{\|f-f_0\|_{2,4}}{\|f-f_0\|_{2,2}} \leq C$$

then:

$$\epsilon(\hat{f},\hat{p},\gamma) \leq O\big(\delta_{n,\zeta} C \|\mu\|_4 \|f-f_0\|_{2,2} + \delta_{n,\zeta}^2\big)$$

Plugging in the bound above to Lemma 2 (which holds irrespective of data re-use or sample splitting or cross-fitting) and applying again the AM-GM inequality yields:

$$\frac{\sigma}{8}\|\hat{f}-f_0\|_{2,2}^2 \leq \frac{1}{\sigma} O\big(\delta_{n,\zeta}^2 C^2 \|\mu\|_4^2 + \|\gamma_{\hat{p},0}^\top(\hat{p}-p_0)\|_{2,2}^2\big)$$

□

C Proof of Thm. 4: Cross-fitted ERM analysis

Let $L_{n,t}$ denote the empirical loss over the samples in the t-th fold and $\hat{p}^{(t)},\hat{\gamma}^{(t)}$ the nuisance functions used on the samples in the k-th fold. For any $t \in [K]$ and conditional on $\hat{p}^{(t)},\hat{\gamma}^{(t)}$, suppose that δ_n upper bounds the critical radius of the function class $\mathcal{G}(\hat{p}^{(t)},\hat{\gamma}^{(t)})$, then by Lemma 11 of Foster & Syrgkanis (2019),[5] if we denote with $\ell_{t,f}(w) = \ell_{\hat{\gamma}^{(t)}}(w;f(x),\hat{p}^{(t)}(x))$, w.p. $1-\zeta$:

$$\Big|L_{n,t}(\hat{f},\hat{p}^{(t)},\hat{\gamma}^{(t)}) - L_{n,t}(f_0,\hat{p}^{(t)},\hat{\gamma}^{(t)}) - (L_D(\hat{f},\hat{p}^{(t)},\hat{\gamma}^{(t)}) - L_D(f_0,\hat{p}^{(t)},\hat{\gamma}^{(t)}))\Big| \leq O\Big(\delta_{n/B,\zeta}\|\ell_{t,f}-\ell_{t,f_0}\|_{2,2} + \delta_{n/B,\zeta}^2\Big)$$

Moreover, we have that by the definition of cross-fitted ERM:

$$\frac{1}{B}\sum_{t=1}^B L_{n,t}(\hat{f},\hat{p}^{(t)},\hat{\gamma}^{(t)}) - L_{n,t}(f_0,\hat{p}^{(t)},\hat{\gamma}^{(t)}) \leq 0$$

Thus we have that w.p. $1-\zeta B$:

$$\frac{1}{B}\sum_{t=1}^B L_D(\hat{f},\hat{p}^{(t)},\hat{\gamma}^{(t)}) - L_D(f_0,\hat{p}^{(t)},\hat{\gamma}^{(t)}) \leq O\left(\delta_{n/B,\zeta}\frac{1}{B}\sum_{t=1}^B \|\ell_{t,f}-\ell_{t,f_0}\|_{2,2} + \delta_{n/B,\zeta}^2\right)$$

Moreover, if we let $\mu(w) = \sup_{\phi,t}\big\|\nabla_\phi \ell(w;\phi,\hat{p}^{(t)}(x))\big\|_2$, then we have by Cauchy-Schwarz inequality:

$$\begin{aligned}
\|\ell_{t,f}-\ell_{t,f_0}\|_{2,2} &\leq \|\mu\|_4\|f-f_0\|_{2,4} + \sqrt{\mathbb{E}\Big[\big((Y-\hat{p}^{(t)}(X))^\top\hat{\gamma}^{(t)}(X)(f(X)-f_0(X))\big)^2\Big]} \\
&\leq \|\mu\|_4\|f-f_0\|_{2,4} + \mathbb{E}\Big[\Big\|(Y-\hat{p}^{(t)}(X))^\top\hat{\gamma}^{(t)}(X)\Big\|_2^2 \|f(X)-f_0(X))\|^2\Big] \\
&\leq \left(\|\mu\|_4 + \mathbb{E}\Big[\Big\|(Y-\hat{p}^{(t)}(X))^\top\hat{\gamma}^{(t)}(X)\Big\|_2^4\Big]^{1/4}\right)\|f-f_0\|_{2,4}
\end{aligned}$$

If we further assume that the function class $\mathcal{F}$ satisfies an ℓ_2/ℓ_4 condition that:

$$\sup_{f\in\mathcal{F}} \frac{\|f-f_0\|_{2,4}}{\|f-f_0\|_{2,2}} \leq C$$

then w.p. $1-\zeta$:

$$\frac{1}{B}\sum_{t=1}^B \epsilon(\hat{f},\hat{p}^{(t)},\hat{\gamma}^{(t)}) \leq O\left(\delta_{n/B,\zeta/B}\frac{1}{B}\sum_{t=1}^B C\left(\|\mu_p\|_4 + \mathbb{E}\Big[\Big\|(Y-\hat{p}(X))^\top\gamma(X)\Big\|_2^4\Big]^{1/4}\right)\|f-f_0\|_{2,2} + \delta_{n/B,\zeta/B}^2\right).$$

Applying Lemma 2 for any $\hat{p}^{(t)},\hat{\gamma}^{(t)}$ and averaging the final inequality we get:

$$\frac{\sigma}{4}\|\hat{f}-f_0\|_{2,2}^2 \leq \frac{1}{B}\sum_{t=1}^B\left(\epsilon(\hat{f},\hat{p}^{(t)},\hat{\gamma}^{(t)}) + \frac{1}{\sigma}\|(\gamma_{f_0,\hat{p}^{(t)}}-\hat{\gamma}^{(t)})^\top(\hat{p}^{(t)}-p_0)\|_{2,2}^2\right).$$

[5] We apply the lemma with $\mathcal{L}_g = g$ and $g \in \mathcal{G}(\hat{p}^{(t)},\hat{\gamma}^{(t)})$ and $g^* = 0$. Then we instantiate the concentration inequality with $g = \ell_{t,\hat{f}} - \ell_{t,f_0} \in \mathcal{G}(\hat{p}^{(t)},\hat{\gamma}^{(t)})$.

Plugging in the bound above to Lemma 2 and applying the AM-GM inequality and Jensen's inequality, yields:

$$\frac{\sigma}{8}\|\hat{f}-f_0\|_{2,2}^2 \leq \frac{1}{\sigma}O\left(\delta_{n/B,\zeta/B}^2 C^2\left(\|\mu\|_4^2+\frac{1}{B}\sum_{t=1}^{B}\sqrt{\mathbb{E}\left[\left\|(Y-\hat{p}^{(t)}(X))^\top\hat{\gamma}^{(t)}(X)\right\|_2^4\right]}\right)\right)$$
$$+\frac{1}{\sigma}O\left(\frac{1}{B}\sum_{t=1}^{B}\|(\gamma_{f_0,\hat{p}^{(t)}}-\hat{\gamma}^{(t)})^\top(\hat{p}^{(t)}-p_0)\|_{2,2}^2\right).$$

D Proof of Thm. 5: Biased SGD analysis

Below, for any integer s, we define the operator norm of any vector $v\in\mathbb{R}^s$ and any tensor T operating on $\mathbb{R}^s$ as

$$\|v\|_{\mathrm{op}} \triangleq \|v\|_2 \quad \text{and} \quad \|T\|_{\mathrm{op}} \triangleq \sup_{v:\|v\|_2=1}\|T[v]\|_{\mathrm{op}}.$$

Recall the definition

$$\nabla(W;\theta,p,\gamma) = \nabla_\theta f_\theta(X)^\top\nabla_\phi\ell_\gamma(W;f_\theta(X),p(X))$$
$$= \nabla_\theta f_\theta(X)^\top(\nabla_\phi\ell(W;f_\theta(X),p(X))+\gamma(X)^\top(Y-p(X))).$$

Observe that since $\mathbb{E}[Y\,|\,X=x]=p_0(x)$, we can write for any γ:

$$\mathcal{L}(\theta;p_0)=\mathbb{E}[\ell(W;f_\theta(X),p_0(X))+(Y-p_0(X))^\top\gamma(X)f_\theta(X)]=\mathbb{E}[\ell_\gamma(W;f_\theta(X),p_0(X))]$$

Thus we also have that:

$$\forall\theta,\gamma:\nabla_\theta\mathcal{L}(\theta;p_0)=\mathbb{E}[\nabla(W;\theta,p_0,\gamma)]$$

Given this observation, we can decompose the gradient that is used in our SGD algorithm into a bias and variance component, when viewed from the perspective of a biased SGD algorithm for the population oracle loss:

$$\nabla(W;\theta,p,\gamma) = \nabla_\theta\mathcal{L}(\theta;p_0)$$
$$+\underbrace{\mathbb{E}[\nabla(W;\theta,p,\gamma)]-\mathbb{E}[\nabla(W;\theta,p_0,\gamma)]}_{\mathbf{b}(\theta,p,\gamma)}+\underbrace{\nabla(W;\theta,p,\gamma)-\mathbb{E}[\nabla(W;\theta,p,\gamma)]}_{\mathbf{n}(W;\theta,p,\gamma)}$$

The following two lemmas bound the gradient bias and noise terms.

Lemma 6 (Gradient bias). *If $\sup_{x,\phi,\pi}\|\mathbb{E}[\nabla_{\pi\pi\phi}\ell(W;\phi,\pi)\,|\,X=x]\|_{\mathrm{op}}\leq M$, then for any parameter vector θ and functions p and γ, we have:*

$$\mathbf{b}(\theta,p,\gamma)=\mathbb{E}[\nabla_\theta f_\theta(X)^\top(\gamma_{f_\theta,p}(X)-\gamma(X))^\top(p(X)-p_0(X))],$$
$$\|\mathbf{b}(\theta,p,\gamma)\|_2\leq\left\|\nabla_\theta f_\theta^\top(\gamma_{f_\theta,p}-\gamma)^\top(p-p_0)\right\|_{2,2}, \quad \textit{and}$$
$$\|\mathbf{b}(\theta,p,\gamma)\|_2\leq\left\|\nabla_\theta f_\theta^\top(q_{f_\theta,p}-\gamma)^\top(p-p_0)\right\|_{2,2}+\frac{M}{2}\|\nabla_\theta f_\theta\|_{F,2}\|p-p_0\|_{2,4}^2.$$

Proof By Taylor's theorem with integral remainder and Lagrange remainder respectively the SGD bias for each parameter i takes the form

$$\mathbf{b}_i(\theta,p,\gamma) = \mathbb{E}[\nabla_i(W;\theta,p,\gamma)]-\mathbb{E}[\nabla_i(W;\theta,p_0,\gamma)]$$
$$= \mathbb{E}[\langle\nabla_\phi\ell_\gamma(W;f_\theta(X),p(X))-\nabla_\phi\ell_\gamma(W;f_\theta(X),p_0(X)),\nabla_{\theta_i}f_\theta(X)\rangle]$$
$$= \mathbb{E}[(p(X)-p_0(X))^\top(\gamma_{f_\theta,p}(X)-\gamma(X))\nabla_{\theta_i}f_\theta(X)]$$
$$= \mathbb{E}[(p(X)-p_0(X))^\top(q_{f_\theta,p}(X)-\gamma(X))\nabla_{\theta_i}f_\theta(X)]$$
$$+\frac{1}{2}\mathbb{E}[\nabla_{\pi\pi\phi}\ell(W;f_\theta(X),\bar{p}(X))[\nabla_{\theta_i}f_\theta(X),p(X)-p_0(X),p(X)-p_0(X)]].$$

Furthermore, our operator norm assumption and Cauchy-Schwarz imply

$$|\mathbf{b}_i(\theta,p,\gamma)|\leq|\mathbb{E}[(p(X)-p_0(X))^\top(q_{f_\theta,p}(X)-\gamma(X))\nabla_{\theta_i}f_\theta(X)]|+\frac{M}{2}\mathbb{E}\left[\|\nabla_{\theta_i}f_\theta(X)\|_2\|p(X)-p_0(X)\|_2^2\right]$$
$$\leq|\mathbb{E}[(p(X)-p_0(X))^\top(q_{f_\theta,p}(X)-\gamma(X))\nabla_{\theta_i}f_\theta(X)]|+\frac{M}{2}\|\nabla_{\theta_i}f_\theta\|_{2,2}\|p-p_0\|_{2,4}^2.$$

Thus, by the triangle inequality and Jensen's inequality we find that

$$\|\mathbf{b}(\theta,p,\gamma)\|_2\leq\left\|\nabla_\theta f_\theta^\top(\gamma_{f_\theta,p}-\gamma)^\top(p-p_0)\right\|_{2,2} \quad \text{and}$$
$$\|\mathbf{b}(\theta,p,\gamma)\|_2\leq\left\|\nabla_\theta f_\theta^\top(q_{f_\theta,p}-\gamma)^\top(p-p_0)\right\|_{2,2}+\frac{M}{2}\|\nabla_\theta f_\theta\|_{F,2}\|p-p_0\|_{2,4}^2.$$

□

Lemma 7 (Gradient Variance). *Define For any parameter θ and functions p and γ,*

$$\sqrt{\mathbb{E}[\|\mathbf{n}(W;\theta,p,\gamma)\|_2^2]}\leq\sigma_0(\theta)+\sqrt{\mathbb{E}[\|\nabla_\theta f_\theta(X)^\top\gamma(X)^\top(Y-p_0(X))\|_2^2]+\left\|\nabla_\theta f_\theta^\top(\gamma_{f_\theta,p}-\gamma)^\top(p-p_0)\right\|_{2,2}^2}.$$

Proof For each $i \in [d]$, define the shorthand

$$\Delta_i = \nabla_{\theta_i} \ell(W; f_\theta(X), p(X)) + \nabla_{\theta_i} f_\theta(X)^\top \gamma(X)^\top (Y - p(X)) - \nabla_{\theta_i} \ell(W; f_\theta(X), p_0(X)) \quad \text{and}$$

$$\begin{aligned} Z_i &= \mathbb{E}[\Delta_i \,|\, X] \\ &= \nabla_{\theta_i} f_\theta(X)^\top (\gamma(X) - \gamma_{f_\theta,p}(X))^\top (p_0(X) - p(X)) \\ &= \nabla_{\theta_i} f_\theta(X)^\top (\gamma(X) - q_{f_\theta,p}(X))^\top (p_0(X) - p(X)) \\ &+ \frac{1}{2} \mathbb{E}[\nabla_{\pi\pi\phi} \ell(W; f_\theta(X), \bar{p}(X))[\nabla_{\theta_i} f_\theta(X), p_0(X) - p(X), p(X) - p_0(X)]] \end{aligned}$$

for some convex combination $\bar{p}(X)$ of $p(X)$ and $p_0(X)$.

We begin by bounding the target expectation using Cauchy-Schwarz

$$\begin{aligned} &\mathbb{E}[\|\mathbf{n}(W; \theta, p, \gamma)\|_2^2] \\ &= \sum_{i \in [d]} \mathrm{Var}[\nabla_{\theta_i} \ell(W; f_\theta(X), p(X)) + \nabla_{\theta_i} f_\theta(X)^\top \gamma(X)^\top (Y - p(X))] \\ &= \sum_{i \in [d]} \mathrm{Var}[\nabla_{\theta_i} \ell(W; f_\theta(X), p_0(X)) + \Delta_i] \\ &= \sigma_0(\theta, p_0)^2 + \sum_{i \in [d]} \mathrm{Var}[\Delta_i] + 2\mathrm{Cov}(\nabla_{\theta_i} \ell(W; f_\theta(X), p_0(X)), \Delta_i) \\ &\leq \sigma_0(\theta, p_0)^2 + \sum_{i \in [d]} \mathrm{Var}[\Delta_i] + 2\sqrt{\mathrm{Var}[\nabla_{\theta_i} \ell(W; f_\theta(X), p_0(X))] \mathrm{Var}[\Delta_i]} \\ &\leq \sigma_0(\theta, p_0)^2 + (\sum_{i \in [d]} \mathrm{Var}[\Delta_i]) + 2\sqrt{\sum_{i \in [d]} \mathrm{Var}[\nabla_{\theta_i} \ell(W; f_\theta(X), p_0(X))] \sum_{i \in [d]} \mathrm{Var}[\Delta_i]} \\ &= (\sigma_0(\theta, p_0) + \sqrt{\sum_{i \in [d]} \mathrm{Var}[\Delta_i]})^2. \end{aligned}$$

We next employ the law of total variance to rewrite the variance terms:

$$\begin{aligned} \sum_{i \in [d]} \mathrm{Var}[\Delta_i] &= \sum_{i \in [d]} \mathrm{Var}[Z_i + \nabla_{\theta_i} f_\theta(X)^\top \gamma(X)^\top (Y - p_0(X))] \\ &= \mathbb{E}[\left\|\nabla_\theta f_\theta(X)^\top \gamma(X)^\top (Y - p_0(X))\right\|_2^2] + \sum_{i \in [d]} \mathrm{Var}[Z_i]. \end{aligned}$$

Finally, we control $\mathrm{Var}[Z_i]$ using Cauchy-Schwarz

$$\sqrt{\sum_{i \in [d]} \mathrm{Var}[Z_i]} \leq \left\|\nabla_\theta f_\theta^\top (\gamma_{f_\theta,p} - \gamma)^\top (p - p_0)\right\|_{2,2}.$$

□

The two claims of Thm. 5 now follow from Theorems 2 and 3 of Ajalloeian & Stich (2020) respectively, with the parameters σ^2 and ζ instantiated with quantities $\sigma^2(\gamma)$ and $\zeta(\gamma)$ of Lemmas 6 and 7.

E Experiment Details and Additional Results

E.1 Synthetic experiment

The synthetic data is generated from a distribution $\mathbb{P}$ that is a mixture of two Gaussians with equal weights. with means at $\pm(r, r, \ldots, r) \in \mathbb{R}^{10}$, where $r \in \mathbb{R}$ controls the separation between the two Gaussian distributions. For each x, the label y is index of the Gaussian from which x was drawn. Given this generative process, the Bayes classifier has the form $p_0(x) = p(y = 1 \,|\, x) = \frac{1}{1 + e^{\theta^T x}}$ for some vector $\theta \in \mathbb{R}^{10}$.

We set $r = 0.25$, and train with gradient descent for 40 epochs, with learning rate 0.3. The λ hyperparameter of the γ-correction was chosen by cross-validation. We repeat the experiments 5 times to measure the mean and standard deviation.

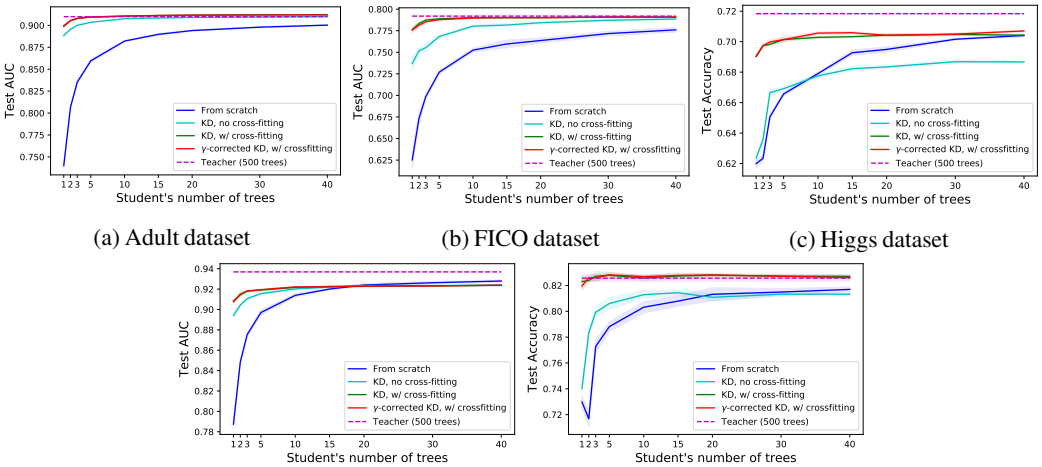
E.2 TABULAR DATA

We use cross-fitting with 10 folds. The λ hyperparameter of the γ-correction was chosen by cross-validation. We repeat the experiments 5 times to measure the mean and standard deviation.

For the overfitting experiment, we use a random forest with 500 trees as the teacher, and a random forest with 1-40 trees as the student. The student is trained to match the class log probability $\log\hat{p}(x)$ of the teacher.

We also evaluate the impact of γ correction compared to without correction (i.e. training on just the teacher's probabilities), especially when the teacher has high bias. We vary the teacher's bias by limited the tree depth in the teacher (from 1 to 20). Lower depth corresponds to more bias. The teacher has 100 trees and the student has 10 trees. For all of the dataset, γ correction successfully reduces the teacher's bias and thus improves the student's performance. The effect is most pronounced when the teacher has large bias (low tree depth).

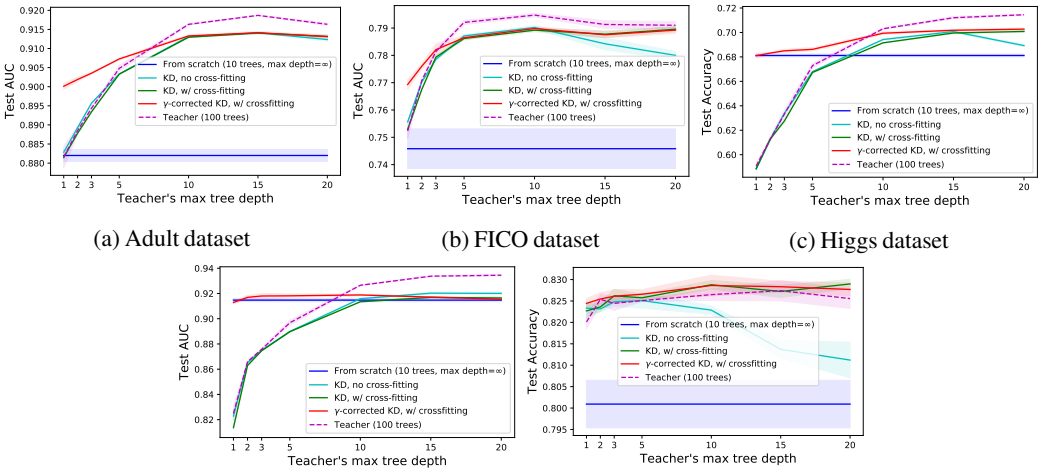
We show the full results for all 5 of the datasets in Figs. 4 and 5.



(a) Adult dataset (b) FICO dataset (c) Higgs dataset

(d) MAGIC dataset (e) StumbleUpon dataset

Figure 4: Comparing knowledge distillation, with and without cross-fitting.



(a) Adult dataset (b) FICO dataset (c) Higgs dataset

(d) MAGIC dataset (e) StumbleUpon dataset

Figure 5: Comparing knowledge distillation, with and without γ correction.

E.3 EXPERIMENT ON IMAGE DATA (CIFAR-10)

We use SGD with initial learning rate 0.1 and momentum 0.9, batch size 128, to train for 200 epochs. We use the standard learning rate decay schedule, where the learning rate is divided by 5 at epoch 60, 120, and 160.