A Deferred Proofs

We now present the proofs of the results from the main paper. In Section A.1, we present the proofs of the average generalization bounds from Section 2. In Section A.2, we prove the high-probability bounds from Section 3. Finally, in Section A.3, we prove the bounds on the information measures from Section 4.

A.1 Proofs for Section 2

We start with Lemma 1.

Proof of Lemma 1. By Jensen's inequality,

$$f_\gamma(\mathbb{E}_{X,Y}[g_1(X,Y)], \mathbb{E}_{X,Y}[g_2(X,Y)]) \leq \mathbb{E}_{X,Y}[f_\gamma(g_1(X,Y), g_2(X,Y))]. \tag{30}$$

By Donsker-Varadhan's variational representation of the KL divergence [43], we have

$$\mathbb{E}_{X,Y}[f_\gamma(g_1(X,Y), g_2(X,Y))] \leq D(P_{XY} \,||\, P_X P_Y) + \log \mathbb{E}_{X,Y'}\left[e^{f_\gamma(g_1(X,Y'), g_2(X,Y'))}\right]. \tag{31}$$

The result follows by noting that $D(P_{XY} \,||\, P_X P_Y) = I(X;Y)$, by re-arranging, and by taking the supremum with respect to γ. □

We now present the proofs of the CMI results given in Section 2. We begin with Remark 1.

Proof of Remark 1. Since each of the random variables is obtained as a function of the previous one, we have the Markov chain

$$W \to \phi_W(\tilde{x}_u) \to \ell(W, \tilde{z}_u). \tag{32}$$

Therefore, the result follows by the data-processing inequality [44, Thm. 2.3.4]. □

Next, we specialize the result of Lemma 1 to the CMI setting in a way that allows for disintegrated CMI results and random subsets.

Corollary 2. *Consider the CMI setting, and fix $\tilde{z}$ and u. As a shorthand, we let $\lambda_u = \ell(\mathcal{A}(\tilde{z}_S, R), \tilde{z}_u)$ denote the matrix of losses incurred on each entry of $\tilde{z}_u$. Let $\lambda_{S_u} = (\lambda_{u_1,S_{u_1}}, \ldots, \lambda_{u_m,S_{u_m}})$. Furthermore, let $\hat{\lambda}_{S_u} = \frac{1}{m}\sum_{i=1}^m \lambda_{u_i,S_{u_i}}$ denote the average loss on the entries of λ selected on the basis of u and S. Let S' be a random variable with the same marginal distribution as S such that λ and S' are independent. Then,*

$$\sup_\gamma \mathbb{E}_{\lambda_u,S_u}\left[f_\gamma(\hat{\lambda}_{S_u}, \hat{\lambda}_{\bar{S}_u})\right] - \log \mathbb{E}_{\lambda_u,S'_u}\left[e^{f_\gamma(\hat{\lambda}_{S'_u}, \hat{\lambda}_{\bar{S}'_u})}\right] \leq I^{\tilde{z},u}(\lambda_u; S_u). \tag{33}$$

Proof. The result follows immediately by applying Lemma 1 with $X = \lambda_u$, $Y = S_u$, $g_1(\lambda_u, S_u) = \hat{\lambda}_{S_u}$, and $g_2(\lambda_u, S_u) = \hat{\lambda}_{\bar{S}_u}$. Since S_u is a discrete random variable, the joint distribution of λ_u, S_u is absolutely continuous with respect to the product of the marginal distributions, that is, the joint distribution of λ_u, S'_u. □

With this, we are ready to derive the results in Theorem 1.

Proof of Theorem 1. Let $f_\gamma(\hat{\lambda}_{S'_u}, \hat{\lambda}_{\bar{S}'_u}) = \gamma(\hat{\lambda}_{\bar{S}'_u} - \hat{\lambda}_{S'_u}) \equiv \gamma\Delta_{S'_u}$, where we use the same notation as in Corollary 2. Due to the symmetry in the definition of the training and test sets, we have that $\Delta_{S'_u} = -\Delta_{\bar{S}'_u}$. This implies that $\mathbb{E}_{S'_u}\left[\Delta_{S'_u}\right] = 0$. Furthermore, $\Delta_{S'_u}$ is the arithmetic average of m independent terms, each with a range of $[-1, 1]$. Thus, $\Delta_{S'_u}$ is a $1/\sqrt{m}$-sub-Gaussian random variable, from which it follows by definition that

$$\log \mathbb{E}_{S'_u}\left[e^{\gamma\Delta_{S'_u}}\right] \leq \frac{\gamma^2}{2m}. \tag{34}$$

Inserting this into (33), we find that

$$\sup_{\gamma} \gamma\Big(\mathbb{E}_{\lambda_u,S_u}\Big[\hat{\lambda}_{S_u}-\hat{\lambda}_{\bar{S}_u}\Big]\Big)-\frac{\gamma^2}{2m}=\frac{m\Big(\mathbb{E}_{\lambda_u,S_u}\Big[\hat{\lambda}_{S_u}-\hat{\lambda}_{\bar{S}_u}\Big]\Big)^2}{2} \leq I^{\tilde{z},u}(\lambda_u;S_u). \tag{35}$$

Since this result is valid for any fixed $\tilde{z}$ and u, it also holds when we average over them. Thus, by re-arranging and averaging, replacing shorthands by their long forms,

$$\mathbb{E}_{\widetilde{Z},U}\Big[\Big|\mathbb{E}_{S,R}\Big[L_{\widetilde{Z}_{S_U}}(\mathcal{A},\widetilde{Z}_S,R)-L_{\widetilde{Z}_{\bar{S}_U}}(\mathcal{A},\widetilde{Z}_S,R)\Big]\Big|\Big] \leq \mathbb{E}_{\widetilde{Z},U}\left[\sqrt{\frac{2I^{\widetilde{Z},U}(\ell(\mathcal{A}(\widetilde{Z}_S,R),\widetilde{Z}_U);S_U)}{m}}\right]. \tag{36}$$

By applying Jensen's inequality, the expectation and absolute value in the left-hand side can be swapped, and by a further use of Jensen's inequality, we can similarly swap the expectation and square root in the right-hand side. Thus, we have shown that

$$\Big|\mathbb{E}_{\widetilde{Z},S,R}\Big[L_{\mathcal{D}}(\mathcal{A},\widetilde{Z}_S,R)-L_{\widetilde{Z}_S}(\mathcal{A},\widetilde{Z}_S,R)\Big]\Big| \leq \mathbb{E}_{\widetilde{Z},U}\left[\sqrt{\frac{2I^{\widetilde{Z},U}(\ell(\mathcal{A}(\widetilde{Z}_S,R),\widetilde{Z}_U);S_U)}{m}}\right] \tag{37}$$

$$\leq \mathbb{E}_U\left[\sqrt{\frac{2I(\ell(\mathcal{A}(\widetilde{Z}_S,R),\widetilde{Z}_U);S_U|\widetilde{Z},U)}{m}}\right]. \tag{38}$$

The right-hand side is an increasing function in the size m of the random subset U [17, Prop. 1]. Hence, we set $m=1$. This establishes the first part of Theorem 1. For the second part of the theorem, we instead consider $f_\gamma(\hat{\lambda}_{S'_u},\hat{\lambda}_{\bar{S}'_u})=\gamma\Delta^2_{\bar{S}'_u}$, with $\gamma\in[0,m/4)$. Since $\Delta_{S'_u}$ is $1/\sqrt{m}$-sub-Gaussian with zero mean, we have [17, Lemma 2]

$$\log \mathbb{E}_{S'_u}\Big[e^{\gamma\Delta^2_{\bar{S}'_u}}\Big] \leq \log\left(1+\frac{8\gamma}{m}\right). \tag{39}$$

By using this in (33), we find that

$$\sup_{\gamma}\gamma\,\mathbb{E}_{\lambda_u,S_u}\left[\left(\hat{\lambda}_{S_u}-\hat{\lambda}_{\bar{S}_u}\right)^2\right]-\log\left(1+\frac{8\gamma}{m}\right) \leq I^{\tilde{z},u}(\lambda_u;S_u). \tag{40}$$

For reasonable values of the involved quantities, the left-hand side is expected to grow as a function of γ. We therefore let $\gamma\to m/4$. Since the bound in (40) holds for the supremum, it also holds for any other choice of γ, including this one. We now have

$$\mathbb{E}_{\lambda_u,S_u}\left[\left(\hat{\lambda}_{S_u}-\hat{\lambda}_{\bar{S}_u}\right)^2\right] \leq \frac{4}{m}\left(I^{\tilde{z},u}(\lambda_u;S_u)+\log 3\right). \tag{41}$$

Averaging over $\widetilde{Z}$ and U, replacing shorthands by their long forms, we obtain

$$\mathbb{E}_{\widetilde{Z},R,S,U}\left[\left(L_{\widetilde{Z}_{S_U}}(\mathcal{A},\widetilde{Z}_S,R)-L_{\widetilde{Z}_{\bar{S}_U}}(\mathcal{A},\widetilde{Z}_S,R)\right)^2\right] \leq \frac{4}{m}\Big(I(\ell(\mathcal{A}(\widetilde{Z}_S,R),\widetilde{Z}_U);S_U|\widetilde{Z},U)+\log 3\Big). \tag{42}$$

We now want to replace the test loss inside the square with the population loss, while still keeping the expectation outside the square. We can do this by using the results of [17, Eq. (116)-Eq. (123)], from which it follows that

$$\mathbb{E}_{\widetilde{Z},R,S}\left[\left(L_{\mathcal{D}}(\mathcal{A},\widetilde{Z}_S,R)-L_{\widetilde{Z}_S}(\mathcal{A},\widetilde{Z}_S,R)\right)^2\right]$$

$$\leq 2\,\mathbb{E}_{\widetilde{Z},R,S,U}\left[\left(L_{\widetilde{Z}_{S_U}}(\mathcal{A},\widetilde{Z}_S,R)-L_{\widetilde{Z}_{S_U}}(\mathcal{A},\widetilde{Z}_S,R)\right)^2\right]+\frac{1}{2m} \tag{43}$$

$$\leq \frac{8}{m}\Big(I(\ell(\mathcal{A}(\widetilde{Z}_S,R),\widetilde{Z}_U);S_U|\widetilde{Z},U)+\log 3\Big)+\frac{1}{2m} \tag{44}$$

$$\leq \frac{8}{m}\Big(\,I(\ell(\mathcal{A}(\widetilde{Z}_S,R),\widetilde{Z}_U);S_U|\widetilde{Z},U)+2\Big). \tag{45}$$

□

Proof of Theorem 2. Consider the CMI setting, with a fixed $\tilde{z}$, u and r. As a shorthand, we let $\tau_u = \ell(\mathcal{A}(\tilde{z}_S, r), \tilde{z}_u)$ denote the matrix of losses incurred on each sample of $\tilde{z}_u$. Let $\tau_{S_u} = (\tau_{u_1,S_{u_1}}, \dots, \tau_{u_m,S_{u_m}})$. Furthermore, let $\hat{\tau}_{S_u} = \frac{1}{m}\sum_{i=1}^m \tau_{u_i,S_i} = L_{\tilde{z}_{S_u}}(\mathcal{A}, \tilde{z}_S, r)$ denote the average loss on the samples of τ indicated by u and S. By following the same steps as in the proof of Theorem 2, we can show that

$$\sup_\gamma \mathbb{E}_{\tau_u,S_u}\left[f_\gamma(\hat{\tau}_{S_u}, \hat{\tau}_{\bar{S}_u})\right] - \log \mathbb{E}_{\tau_u,S'_u}\left[e^{f_\gamma(\hat{\tau}_{S'_u}, \hat{\tau}_{\bar{S}'_u})}\right] \le I^{\tilde{z},u,r}(\tau_u; S_u). \tag{46}$$

Let $f_\gamma(\hat{\tau}_{S'_u}, \hat{\tau}_{\bar{S}'_u}) = \gamma(\hat{\tau}_{\bar{S}'_u} - \hat{\tau}_{S'_u}) = \gamma\Xi_{S'_u}$. By the same argument as in the proof of Theorem 1, we conclude that $\Xi_{S'_u}$ is $1/\sqrt{m}$-sub-Gaussian. Thus, (34) holds with $\Xi_{S'_u}$ in place of $\Delta_{S'_u}$. Inserting this into (46), we find that

$$\sup_\gamma \gamma\big(\mathbb{E}_{\tau_u,S_u}\left[\hat{\tau}_{S_u} - \hat{\tau}_{\bar{S}_u}\right]\big) - \frac{\gamma^2}{2m} = \frac{m\big(\mathbb{E}_{\tau_u,S_u}\left[\hat{\tau}_{S_u} - \hat{\tau}_{\bar{S}_u}\right]\big)^2}{2} \le I^{\tilde{z},u,r}(\tau_u; S_u). \tag{47}$$

Finally, by re-arranging, replacing shorthands by their long forms, averaging over $\widetilde{Z}$, S, and R, and using Jensen's inequality to move the expectation inside the absolute value, we find that

$$\left|\mathbb{E}_{\widetilde{Z},S,R}\Big[L_{\mathcal{D}}(\mathcal{A}, \widetilde{Z}_S, R) - L_{\widetilde{Z}_S}(\mathcal{A}, \widetilde{Z}_S, R)\Big]\right| \le \mathbb{E}_{\widetilde{Z},U,R}\left[\sqrt{\frac{2I^{\widetilde{Z},U,R}(\ell(\mathcal{A}(\widetilde{Z}_S, R), \widetilde{Z}_U); S_U)}{m}}\right]. \tag{48}$$

The desired bound in (8) follows by setting $m = 1$, and (9) follows by Jensen's inequality. □

Proof of Theorem 3. We need to use the following two concentration results that are implicitly used in [16] and more explicitly stated in [18].

Lemma 3. *Consider a binary random variable X satisfying $P(X = a) = P(X = b) = 1/2$ where $a, b \in [0, 1]$. Let $\bar{X} = a + b - X$ be the complement of X in $\{a, b\}$. Assume that γ_1 and γ_2 satisfy $\gamma_1(1 - \gamma_2) + (e^{\gamma_1} - 1 - \gamma_1)(1 + \gamma_2^2) \le 0$. Then,*

$$\mathbb{E}_X\left[e^{\gamma_1\left(X - \gamma_2\bar{X}\right)}\right] \le 1. \tag{49}$$

Furthermore, assume that $a = 0$. Then,

$$\lim_{\gamma\to\infty} \mathbb{E}_X\left[e^{\log 2(\bar{X} - \gamma X)}\right] \le 1. \tag{50}$$

Proof. The first part follows by [13, Eq. (7)]. For the second part, note that

$$\mathbb{E}_X\left[e^{\log 2(\bar{X} - \gamma X)}\right] = \frac{e^{b\log 2} + e^{-b\gamma\log 2}}{2}. \tag{51}$$

If $b = 0$, the right-hand side of (51) equals 1 for all γ. If $b \neq 0$, we have

$$\lim_{\gamma\to\infty} \frac{e^{b\log 2} + e^{-b\gamma\log 2}}{2} = \frac{e^{b\log 2}}{2} \le \frac{e^{\log 2}}{2} = 1, \tag{52}$$

where the last inequality follows because $b \in [0, 1]$. □

We now proceed with the proof of Theorem 3. Fix $\tilde{z}$ and u. To apply Corollary 2, we set $f_\gamma(\hat{\lambda}_{S'_u}, \hat{\lambda}_{\bar{S}'_u}) = m\gamma_1(\hat{\lambda}_{S'_u} - \gamma_2\hat{\lambda}_{\bar{S}'_u})$, where we use the same notation as in Corollary 2. Since the elements of S'_u are independent,

$$\mathbb{E}_{S'_u}\left[e^{m\gamma_1(\hat{\lambda}_{S'_u} - \gamma_2\hat{\lambda}_{\bar{S}'_u})}\right] = \prod_{i=1}^m \mathbb{E}_{S'_{u_i}}\left[e^{\gamma_1\left(\lambda_{u_i,S'_{u_i}} - \gamma_2\lambda_{u_i,\bar{S}'_{u_i}}\right)}\right] \le 1 \tag{53}$$

where the last inequality follows from (49). Hence,

$$\sup_\gamma \mathbb{E}_{\lambda_u,S_u}\left[n\gamma_1(\hat{\lambda}_{S_u} - \gamma_2\hat{\lambda}_{\bar{S}_u})\right] \le I^{\tilde{z},u}(\lambda_u; S_u). \tag{54}$$

Since (54) holds when we take the supremum over γ, it also holds for any other choice of γ. For now, let $\gamma = (\gamma_1, \gamma_2)$ be any pair of parameters that satisfy the constraint of Theorem 3. Averaging over $\widetilde{Z}$ and U, replacing shorthands by their long forms, we get

$$\mathbb{E}_{\widetilde{Z},S,R}\Big[L_{\mathcal{D}}(\mathcal{A},\widetilde{Z}_S,R)\Big] \le \gamma_2\,\mathbb{E}_{\widetilde{Z},S,R}\Big[L_{\widetilde{Z}_S}(\mathcal{A},\widetilde{Z}_S,R)\Big] + \frac{I(\ell(\mathcal{A}(\widetilde{Z}_S,R),\widetilde{Z}_U);S_U|\widetilde{Z},U)}{m\gamma_1}. \quad (55)$$

Since the right-hand side is an increasing function of m, the tightest result is obtained for $m = 1$. Making this choice and optimizing the parameters, we obtain (11).

We now turn to (12). Fix $\tilde{z}$ and u. Now, set $f_\gamma(\hat{\lambda}_{S'_u},\hat{\lambda}_{\bar{S}'_u}) = m\log 2(\hat{\lambda}_{\bar{S}'_u} - \gamma\hat{\lambda}_{S'_u})$. Then, (33) implies that

$$\mathbb{E}_{\lambda_u,S_u}\Big[m\log 2(\hat{\lambda}_{\bar{S}_u} - \gamma\hat{\lambda}_{S_u})\Big] - \log\mathbb{E}_{\lambda_u,S'_u}\Big[e^{m\log 2(\hat{\lambda}_{\bar{S}'_u}-\gamma\hat{\lambda}_{S'_u})}\Big] \le I^{\tilde{z},u}(\lambda_u;S_u). \quad (56)$$

In view of (50), we let $\gamma\to\infty$. Note that the assumption that $\hat{L}=0$ implies that $\lambda_{i,S_i}=0$ with probability 1. Thus, by the independence of the elements of S'_u, (50) implies that

$$\lim_{\gamma\to\infty}\mathbb{E}_{\lambda_u,S'_u}\left[e^{m\log 2(\hat{\lambda}_{\bar{S}'_U}-\gamma\hat{\lambda}_{S'_U})}\right] = \lim_{\gamma\to\infty}\prod_{i=1}^{m}\mathbb{E}_{\lambda_u,S'_{U_i}}\left[e^{\log 2\left(\lambda_{U_i,\bar{S}'_{U_i}}-\gamma\lambda_{U_i,S'_{U_i}}\right)}\right] \le 1. \quad (57)$$

We now average over $\widetilde{Z}$ and U. By the assumption that $\hat{L}=0$, we have

$$\mathbb{E}_{\widetilde{Z},U,\lambda_U,S_U}\Big[m\log 2(\hat{\lambda}_{\bar{S}_u} - \gamma\hat{\lambda}_{S_u})\Big] = \mathbb{E}_{\widetilde{Z},U,\lambda_U,S_U}\Big[m\log 2(\hat{\lambda}_{\bar{S}_u})\Big]. \quad (58)$$

This means that we can discard the second term in (56) when $\gamma\to\infty$. We finally establish the desired result by setting $m=1$. □

Proof of Lemma 2. Let $Y_1,\dots,Y_n$ be independent Bernoulli random variables satisfying $\mathbb{E}[Y_i]=\mu_i$. It follows from [30, Lemma 1] that, for every convex function f,

$$\mathbb{E}[f(X_1,\dots,X_n)] \le \mathbb{E}[f(Y_1,\dots,Y_n)]. \quad (59)$$

Next, let $Y=\sum_{i=1}^n Y_i$ and let $\mu=\sum_{i=1}^n\mu_i/n$. Also, let $\bar{Y}\sim\mathrm{Bin}(n,\mu)$ be a Binomial random variable. Then, for any strictly convex function g, we have [31, Thm. 3]

$$\mathbb{E}[g(Y)] \le \mathbb{E}\big[g(\bar{Y})\big]. \quad (60)$$

Now, let h be the linear function $h(X_1,\dots,X_n)=\sum_{i=1}^n X_i = X$. Notice that the strict convexity of g implies that $g\circ h$ is convex. It then follows from (59) with $f=g\circ h$ that

$$\mathbb{E}[g(X)] = \mathbb{E}[g\circ h(X_1,\dots,X_n)] \le \mathbb{E}[g\circ h(Y_1,\dots,Y_n)] = \mathbb{E}[g(Y)]. \quad (61)$$

Combining (60) and (61), we conclude that

$$\mathbb{E}[g(X)] \le \mathbb{E}\big[g(\bar{Y})\big]. \quad (62)$$

Now, we set $g(x)=\exp(nd_\gamma(x/n\,||\,\mu))$, which is strictly convex. Then, it follows from (62) that

$$\mathbb{E}[\exp(nd_\gamma(X/n\,||\,\mu))] \le \mathbb{E}\big[\exp(nd_\gamma(\bar{Y}/n\,||\,\mu))\big]. \quad (63)$$

Note that $X/n=\hat{\mu}$. Next, by [29, Eq. (17)], we have

$$\mathbb{E}\big[\exp(nd_\gamma(\bar{Y}/n\,||\,\mu))\big] \le 1. \quad (64)$$

Combining (63) and (64), we obtain the desired result. □

Proof of Theorem 4 and Theorem 5. The results in Theorem 4 and Theorem 5 follow as a special case of Theorem 10, which is stated and proven in Appendix B. □

Proof of Theorem 6. With the standard convention that $0\log 0=0$, which is motivated by continuity, we get

$$d\Big(0\,||\,\frac{p}{2}\Big) = \log\frac{1}{1-\frac{p}{2}}. \quad (65)$$

Then, it follows from (19) that $d^{-1}(0,c)=2-2e^{-c}$. Combining this with (20), we obtain (23). □

A.2 Proofs for Section 3

We now turn to the proof of the high-probability bound in Theorem 7.

Proof of Theorem 7. Let the size of the subset U be n. Let $f_\gamma(\cdot,\cdot)$ be a function that is jointly convex in its arguments. Now, consider the random variables $\lambda \sim P_{\lambda|\widetilde{Z}S}$ and $\lambda' \sim P_{\lambda|\widetilde{Z}}$. We use the notation from Corollary 2, and set $\lambda_S = (\lambda_{1,S_1}, \ldots, \lambda_{n,S_n})$, $\hat{\lambda}_S = \sum_{i=1}^n \lambda_{i,S_i}/n$ and $\hat{\lambda}_{\bar{S}} = \sum_{i=1}^n \lambda_{i,\bar{S}_i}/n$. Then, by Jensen's inequality,

$$f_\gamma\Big(\mathbb{E}_R\Big[L_{\widetilde{Z}_S}(\mathcal{A},\widetilde{Z}_S,R)\Big], \mathbb{E}_R\Big[L_{\widetilde{Z}_{\bar{S}}}(\mathcal{A},\widetilde{Z}_S,R)\Big]\Big) = f_\gamma\Big(\mathbb{E}_\lambda\Big[\hat{\lambda}_S\Big], \mathbb{E}_\lambda\Big[\hat{\lambda}_{\bar{S}}\Big]\Big) \tag{66}$$

$$\leq \mathbb{E}_\lambda\Big[f_\gamma(\hat{\lambda}_S,\hat{\lambda}_{\bar{S}})\Big]. \tag{67}$$

By Donsker-Varadhan's variational representation of the KL divergence [43],

$$\mathbb{E}_\lambda\Big[f_\gamma(\hat{\lambda}_S,\hat{\lambda}_{\bar{S}})\Big] \leq D(P_{\lambda|\widetilde{Z}S}\,||\,P_{\lambda|\widetilde{Z}}) + \log \mathbb{E}_{\lambda'}\Big[\exp(f_\gamma(\hat{\lambda}'_S,\hat{\lambda}'_{\bar{S}}))\Big]. \tag{68}$$

By Markov's inequality, we conclude that with probability at least $1-\delta$ under the draw of $\widetilde{Z}$ and S,

$$D(P_{\lambda|\widetilde{Z}S}\,||\,P_{\lambda|\widetilde{Z}}) + \log \mathbb{E}_{\lambda'}\Big[\exp(f_\gamma(\hat{\lambda}'_S,\hat{\lambda}'_{\bar{S}}))\Big] \tag{69}$$

$$\leq D(P_{\lambda|\widetilde{Z}S}\,||\,P_{\lambda|\widetilde{Z}}) + \log\frac{1}{\delta}\,\mathbb{E}_{\lambda',\widetilde{Z},S}\Big[\exp(f_\gamma(\hat{\lambda}'_S,\hat{\lambda}'_{\bar{S}}))\Big] \tag{70}$$

$$= D(P_{\lambda|\widetilde{Z}S}\,||\,P_{\lambda|\widetilde{Z}}) + \log\frac{1}{\delta}\,\mathbb{E}_{\lambda,\widetilde{Z},S'}\Big[\exp(f_\gamma(\hat{\lambda}_{S'},\hat{\lambda}_{\bar{S}'}))\Big]. \tag{71}$$

In (71), S' is a copy of S that is independent from λ. The step from (70) to (71) relies on the observation that λ' is independent of S but has the same joint distribution with $\widetilde{Z}$ as λ does. Now, let $f_\gamma(\hat{\lambda}_{S'},\hat{\lambda}_{\bar{S}'}) = \frac{(n-1)}{2}(\hat{\lambda}_{\bar{S}'} - \hat{\lambda}_{S'})^2 \equiv \frac{(n-1)}{2}\Delta^2_{S'}$. Due to the symmetry in the definition of the training and test sets, we have that $\Delta_{S'} = -\Delta_{\bar{S}'}$. This implies that $\mathbb{E}_{S'}[\Delta_{S'}] = 0$. Furthermore, $\Delta_{S'}$ is the arithmetic average of n independent terms, each with a range of $[-1,1]$. Thus, $\Delta_{S'}$ is a $1/\sqrt{n}$-sub-Gaussian random variable, from which it follows that [45, Thm. 2.6.(IV)]

$$\log \mathbb{E}_{S'}\Big[e^{\frac{(n-1)}{2}\Delta^2_{S'}}\Big] \leq \log\big(\sqrt{n}\big). \tag{72}$$

Inserting this into (71) and combining the result with (67), we obtain

$$\frac{n-1}{2}\,\mathbb{E}_R\Big[(L_{\widetilde{Z}_{\bar{S}}}(\mathcal{A},\widetilde{Z}_S,R) - L_{\widetilde{Z}_S}(\mathcal{A},\widetilde{Z}_S,R))^2\Big] \leq D(P_{\lambda|\widetilde{Z}S}\,||\,P_{\lambda|\widetilde{Z}}) + \log\frac{\sqrt{n}}{\delta}. \tag{73}$$

By Jensen's inequality, this implies that

$$\frac{n-1}{2}\Big(\mathbb{E}_R\Big[L_{\widetilde{Z}_{\bar{S}}}(\mathcal{A},\widetilde{Z}_S,R) - L_{\widetilde{Z}_S}(\mathcal{A},\widetilde{Z}_S,R)\Big]\Big)^2 \leq D(P_{\lambda|\widetilde{Z}S}\,||\,P_{\lambda|\widetilde{Z}}) + \log\frac{\sqrt{n}}{\delta} \tag{74}$$

from which the result in (24) follows.

To prove (25), let $f_\gamma(\hat{\lambda}_{S'},\hat{\lambda}_{\bar{S}'}) = nd(\hat{\lambda}_{S'}\,||\,(\hat{\lambda}_{S'}+\hat{\lambda}_{\bar{S}'})/2)$. We now note that $\mathbb{E}_{S'}\Big[\hat{\lambda}_{S'}\Big] = \hat{\lambda}$, where $\hat{\lambda} = \sum_{i=1}^n(\lambda_{i,0}+\lambda_{i,1})/2n$. For any s', this can be written as $\hat{\lambda} = (\hat{\lambda}_{s'}+\hat{\lambda}_{\bar{s}'})/2$ due to symmetry. Therefore, by [22, Thm. 1],

$$\log \mathbb{E}_{S'}\Big[e^{nd(\hat{\lambda}_{S'}\,||\,(\hat{\lambda}_{S'}+\hat{\lambda}_{\bar{S}'})/2)}\Big] \leq \log\Big(\sqrt{2n}\Big). \tag{75}$$

Again, inserting this into (71) and combining the result with (67), we obtain

$$d\left(\mathbb{E}_R\Big[L_{\widetilde{Z}_S}(\mathcal{A},\widetilde{Z}_S,R)\Big]\;||\;\mathbb{E}_R\left[\frac{L_{\widetilde{Z}_S}(\mathcal{A},\widetilde{Z}_S,R)+L_{\widetilde{Z}_{\bar{S}}}(\mathcal{A},\widetilde{Z}_S,R)}{2}\right]\right)$$

$$\leq \frac{D(P_{\lambda|\widetilde{Z}S}\,||\,P_{\lambda|\widetilde{Z}}) + \log\frac{2\sqrt{n}}{\delta}}{n}, \tag{76}$$

which gives the desired result. □

A.3 Proofs for Section 4

Before proceeding with the proof of Theorem 8, we need the following lemma.

Lemma 4. *Let $g_{\mathcal{F}}(\cdot)$ denote the growth function of the function class $\mathcal{F}$, i.e., $g_{\mathcal{F}}(m)$ is the maximum number of different ways in which a data set of size m can be classified using functions from $\mathcal{F}$. For any function class $\mathcal{F}$ with range $\{0,\dots,N-1\}$ and Natarajan dimension d_N,*

$$g_{\mathcal{F}}(m) \leq \sum_{i=0}^{d_N} \binom{m}{i}\binom{N}{2}^i \leq \begin{cases} N^{d_N+1}, & m < d_N+1, \\ \left(\binom{N}{2}\frac{em}{d_N}\right)^{d_N}, & m \geq d_N+1. \end{cases} \tag{77}$$

Proof. The first inequality follows from [46, Cor. 5] and the second follows from [39, Lemma 10]. □

Proof of Theorem 8. We begin with (26), the proof of which is similar to that of [17, Thm. 4.1], which, however, focuses on the VC dimension. Let $f(\mathcal{A}(\widetilde{Z}_S, R), \widetilde{Z})$ denote the predictions of the algorithm on the supersample. Given $\widetilde{Z}$, the losses induced by the algorithm are a function of the predictions. Therefore, by the data-processing inequality, [44, Thm. 2.3.4]

$$I(\ell(\mathcal{A}(\widetilde{Z}_S, R), \widetilde{Z}); S|\widetilde{Z}) \leq I(f(\mathcal{A}(\widetilde{Z}_S, R), \widetilde{Z}); S|\widetilde{Z}). \tag{78}$$

Let $F(\widetilde{Z})$ denote the set of all possible values taken by $f(\mathcal{A}(\widetilde{Z}_S, R), \widetilde{Z})$ by varying S and R but keeping $\widetilde{Z}$ fixed. Then,

$$I(f(\mathcal{A}(\widetilde{Z}_S, R), \widetilde{Z}); S|\widetilde{Z}) \leq H(f(\mathcal{A}(\widetilde{Z}_S, R), \widetilde{Z})|\widetilde{Z}) \tag{79}$$

$$\leq \sup_{\widetilde{Z}} \log \left|F(\widetilde{Z})\right|. \tag{80}$$

Here, $H(f(\mathcal{A}(\widetilde{Z}_S, R), \widetilde{Z})|\widetilde{Z})$ denotes the conditional entropy of $f(\mathcal{A}(\widetilde{Z}_S, R), \widetilde{Z})$ given $\widetilde{Z}$. Since the learning algorithm implements a function from $\mathcal{F}$, and $\widetilde{Z}$ consists of $2n$ samples, we conclude that $\left|F(\widetilde{Z})\right|$ can be no larger than $g_{\mathcal{F}}(2n)$. Using Lemma 4, we note that, if $2n \geq d_N + 1$,

$$\sup_{\widetilde{Z}} \log \left|F(\widetilde{Z})\right| \leq \log g_{\mathcal{F}}(2n) \leq d_N \log\left(\binom{N}{2}\frac{2en}{d_N}\right). \tag{81}$$

This concludes the proof of (26).

We now turn to (27). First, by Jensen's inequality,

$$D(P_{\lambda|\widetilde{Z}S} \,||\, P_{\lambda|\widetilde{Z}}) = \mathbb{E}_{P_{\lambda|\widetilde{Z}S}}\left[\log \frac{P_{\lambda|\widetilde{Z}S}}{P_{\lambda|\widetilde{Z}}}\right] \leq \log \mathbb{E}_{P_{\lambda|\widetilde{Z}S}}\left[\frac{P_{\lambda|\widetilde{Z}S}}{P_{\lambda|\widetilde{Z}}}\right]. \tag{82}$$

By Markov's inequality we conclude that, with probability at least $1-\delta$ under the draw of $(\widetilde{Z}, S)$,

$$\log \mathbb{E}_{P_{\lambda|\widetilde{Z}S}}\left[\frac{P_{\lambda|\widetilde{Z}S}}{P_{\lambda|\widetilde{Z}}}\right] \leq \log\left(\frac{1}{\delta}\,\mathbb{E}_{P_{\lambda\widetilde{Z}S}}\left[\frac{P_{\lambda|\widetilde{Z}S}}{P_{\lambda|\widetilde{Z}}}\right]\right). \tag{83}$$

Since λ is a discrete random variable, its probability mass function is bounded by 1. Hence,

$$\log\left(\frac{1}{\delta}\,\mathbb{E}_{P_{\lambda\widetilde{Z}S}}\left[\frac{P_{\lambda|\widetilde{Z}S}}{P_{\lambda|\widetilde{Z}}}\right]\right) \leq \log\left(\frac{1}{\delta}\,\mathbb{E}_{P_{\lambda\widetilde{Z}}}\left[\frac{1}{P_{\lambda|\widetilde{Z}}}\right]\right). \tag{84}$$

By upper-bounding the average over $\widetilde{Z}$ by its supremum, we find that

$$\log\left(\frac{1}{\delta}\,\mathbb{E}_{P_{\lambda\widetilde{Z}}}\left[\frac{1}{P_{\lambda|\widetilde{Z}}}\right]\right) \leq \log\left(\frac{1}{\delta}\sup_{\widetilde{Z}}\,\mathbb{E}_{P_{\lambda|\widetilde{Z}}}\left[\frac{1}{P_{\lambda|\widetilde{Z}}}\right]\right). \tag{85}$$

Let $L(\widetilde{Z})$ denote the set of all possible values that λ can take given $\widetilde{Z}$. Then,

$$\log\left(\frac{1}{\delta}\sup_{\widetilde{z}}\mathbb{E}_{P_{\lambda|\widetilde{z}}}\left[\frac{1}{P_{\lambda|\widetilde{Z}}}\right]\right) = \log\left(\frac{1}{\delta}\sup_{\widetilde{z}}\sum_{\lambda\in L(\widetilde{Z})} P_{\lambda|\widetilde{z}}(\lambda)\frac{1}{P_{\lambda|\widetilde{z}}(\lambda)}\right) \tag{86}$$

$$= \sup_{\widetilde{z}}\log\frac{\left|L(\widetilde{Z})\right|}{\delta}. \tag{87}$$

Finally, since the map from $F(\widetilde{Z})$ to $L(\widetilde{Z})$ induced by $\ell(\cdot,\cdot)$ is surjective,

$$\sup_{\widetilde{z}}\log\frac{\left|L(\widetilde{Z})\right|}{\delta} \leq \sup_{\widetilde{z}}\log\frac{\left|F(\widetilde{Z})\right|}{\delta}. \tag{88}$$

Again, note that $\left|F(\widetilde{Z})\right|$ can be no larger than the growth function of $\mathcal{F}$ evaluated at $2n$, i.e., $g_{\mathcal{F}}(2n)$. Therefore, if $2n \geq d_N + 1$, it follows from Lemma 4 that

$$\sup_{\widetilde{z}}\log\left|F(\widetilde{Z})\right| \leq \log g_{\mathcal{F}}(2n) \leq d_N \log\left(\binom{N}{2}\frac{2en}{d_N}\right). \tag{89}$$

The desired result now follows by combining (82)-(89). □

Proof of Corollary 1. By Jensen's inequality,

$$\frac{1}{n}\sum_{i=1}^{n}\sqrt{2I(\ell(\mathcal{A}(\widetilde{Z}_S,R),\widetilde{Z}_i);S_i|\widetilde{Z})} \leq \sqrt{\frac{1}{n}\sum_{i=1}^{n}2I(\ell(\mathcal{A}(\widetilde{Z}_S,R),\widetilde{Z}_i);S_i|\widetilde{Z})}. \tag{90}$$

From the independence of the S_i, it follows that

$$\frac{1}{n}\sum_{i=1}^{n}I(\ell(\mathcal{A}(\widetilde{Z}_S,R),\widetilde{Z}_i);S_i|\widetilde{Z}) \leq \frac{I(\ell(\mathcal{A}(\widetilde{Z}_S,R),\widetilde{Z});S|\widetilde{Z})}{n}. \tag{91}$$

We first combine (5), (90), and (91) to upper-bound the samplewise information term in (5) by its full-sample counterpart. Then, to establish the result in (28), we use (26) to upper-bound the full-sample e-CMI in terms of the Natarajan dimension.

To establish (29), we first use (25) and (27). Since both of these inequalities are probabilistic and hold with probability at least $1-\delta$, by the union bound, they both hold with probability at least $1-2\delta$. To obtain the statement in Corollary 1, we replace δ with $\delta/2$. □

B Additional Theoretical Results

In this section, we present some additional theoretical results. In Section B.1, we present an analogue of Theorem 4 given in terms of the regular mutual information rather than the e-CMI. In Section B.2, we show how to tighten the bounds in Theorem 4 and 5 by introducing affine transformations. In Section B.3, we present a version of Theorem 7 that holds with high probability also over the draw of R. Finally, in Section B.4, we performed a more detailed comparison of our bounds to results found in the literature.

B.1 Binary KL Bound with Samplewise Mutual Information

In this section, we derive a binary KL bound in terms of the samplewise mutual information between the learning algorithm's output and the training data. This can be seen as an average, samplewise version of what in the PAC-Bayesian literature is sometimes referred to as Seeger's bound [4, Sec. 3.2.3]. To the best of our knowledge, neither this samplewise bound nor its full-sample analogue have been explicitly stated in the literature, although the necessary ingredients for deriving the full-sample bound are already present in [29]. Note that, since we do not consider the CMI setting in Theorem 9, the definitions of $\hat{L}$ and $L_{\mathcal{D}}$ differ from the ones used in the rest of the paper.

Theorem 9 (Binary KL mutual information bound)**.** *Let Z be an n-dimensional vector with entries generated independently according to $\mathcal{D}$. Furthermore, let $\hat{L} = \mathbb{E}_{Z,R}[L_Z(\mathcal{A}, Z, R)]$ and $L_{\mathcal{D}} = \mathbb{E}_{Z,R}[L_{\mathcal{D}}(\mathcal{A}, Z, R)]$. Then,*

$$d(\hat{L} \,||\, L_{\mathcal{D}}) \leq \frac{1}{n} \sum_{i=1}^{n} I(\mathcal{A}(Z, R); Z_i) \tag{92}$$

where $d(\hat{L} \,||\, L_{\mathcal{D}})$ is the binary KL divergence, i.e., the KL divergence between two Bernoulli distributions with parameters $\hat{L}$ and $L_{\mathcal{D}}$, respectively.

Proof of Theorem 9. Let $F = \mathcal{A}(Z, R)$ denote the output of the learning algorithm, and let $L_{\mathcal{D}}(f) = \mathbb{E}_Z[\ell(f, Z)]$ with $Z \sim \mathcal{D}$. Let $Z' \sim \mathcal{D}$ be independent of F. For any fixed f, we have $\mathbb{E}_{Z'}[\ell(f, Z')] = L_{\mathcal{D}}(f)$. Therefore, by Lemma 2,

$$\mathbb{E}_{F,Z'}\left[e^{d_\gamma(\ell(F,Z') \,||\, L_{\mathcal{D}}(F))}\right] \leq 1. \tag{93}$$

We now set $X = F$, $Y = Z_i$, $g_1(F, Z_i) = \ell(F, Z_i)$, $g_2(F, Z_i) = L_{\mathcal{D}}(F)$, and $f_\gamma(\cdot, \cdot) = d_\gamma(\cdot \,||\, \cdot)$, and note that (93) implies that $\xi_\gamma \leq 0$ in Lemma 1. Hence, we conclude that

$$\sup_\gamma \mathbb{E}_{F,Z_i}[d_\gamma(\ell(F, Z_i) \,||\, L_{\mathcal{D}}(F))] \leq I(F; Z_i). \tag{94}$$

By decomposing the training loss as $L_Z(\mathcal{A}, Z, R) = \frac{1}{n}\sum_{i=1}^n \ell(F, Z_i)$ and using (14), we have

$$d(\mathbb{E}_{F,Z}[L_Z(\mathcal{A},Z,R)] \,||\, \mathbb{E}_{F,Z}[L_{\mathcal{D}}(F)]) = \sup_\gamma d_\gamma\left(\frac{1}{n}\sum_{i=1}^n \mathbb{E}_{F,Z_i}[\ell(F, Z_i)], \frac{1}{n}\sum_{i=1}^n \mathbb{E}_{F,Z_i}[L_{\mathcal{D}}(F)]\right). \tag{95}$$

Since $d_\gamma(\cdot \,||\, \cdot)$ is jointly convex in its arguments, Jensen's inequality implies that

$$\sup_\gamma d_\gamma\left(\frac{1}{n}\sum_{i=1}^n \mathbb{E}_{F,Z_i}[\ell(F, Z_i)\,, \frac{1}{n}\sum_{i=1}^n \mathbb{E}_{F,Z_i}[L_{\mathcal{D}}(F)]\right) \leq \sup_\gamma \frac{1}{n}\sum_{i=1}^n \mathbb{E}_{F,Z_i}[d_\gamma(\ell(F, Z_i), L_{\mathcal{D}}(F))]. \tag{96}$$

Combining this with (94), we obtain

$$d(\mathbb{E}_{F,Z}[L_Z(\mathcal{A}, Z, R)] \;||\; \mathbb{E}_{F,Z}[L_{\mathcal{D}}(F)]) \leq \frac{1}{n}\sum_{i=1}^n I(F; Z_i) \tag{97}$$

from which the result follows. □

To convert this result into an upper bound on the population loss, one needs to numerically invert the binary KL divergence. This can be done by evaluating [47]

$$L_{\mathcal{D}} \leq \sup\left\{L'_{\mathcal{D}} \in [0, 1] : d(\hat{L} \,||\, L'_{\mathcal{D}}) \leq \frac{1}{n}\sum_{i=1}^n I(\mathcal{A}(Z, R); Z_i)\right\}. \tag{98}$$

We now rewrite (92) to make the connection to standard PAC-Bayesian results [27, 29] more apparent. Let $F = \mathcal{A}(Z, R)$, and let $P_{F|Z}$ denote the stochastic kernel that represents the randomized learning algorithm, that is, the PAC-Bayesian posterior. Furthermore, let P_F denote the corresponding marginal distribution, and let $P_Z = \mathcal{D}^n$ denote the data distribution. Finally, let $P_{F|Z_i}$ denote the resulting distribution when we marginalize $P_{F|Z}$ over all training examples except the ith. By the golden formula [48, Eq. (8.7)], we can upper-bound the mutual information by replacing the true marginal distribution in the KL divergence with some auxiliary distribution. Specifically,

$$I(F; Z_i) \leq D(P_{F|Z_i} P_{Z_i} \,||\, Q_F P_{Z_i}), \tag{99}$$

where Q_F is an arbitrary distribution on $\mathcal{F}$ satisfying $P_{F|Z_i}$ is absolutely continuous with respect to Q_F. Here, Q_F corresponds to the PAC-Bayesian prior. Thus, Theorem 9 implies that

$$d(\hat{L} \,||\, L_{\mathcal{D}}) \leq \frac{1}{n}\sum_{i=1}^n D(P_{F|Z_i} P_{Z_i} \,||\, Q_F P_{Z_i}). \tag{100}$$

Note that in all bounds reported in the rest of the paper, one can replace the true marginal with an auxiliary distribution. In some situations, this leads to more tractable bounds.

One commonly used approach to tighten PAC-Bayesian bounds is to consider data-dependent priors [25]. This can be achieved through techniques such as differential privacy [49] or data splitting, where the training samples are divided into one part used for evaluating the bound and one part for constructing the prior [50, 51, 52]. As noted by [18], the CMI setting can be seen as a way to automatically obtain data-dependent priors.

B.2 Affine Transformations of the Arguments in the Binary KL Bound

As mentioned in Section 2.3, the binary KL bounds in Theorem 4 and Theorem 5 can be tightened by considering affine transformations of the arguments of the arguments of $d(\cdot \,||\, \cdot)$. We present this in the following theorem.

Theorem 10 (Affine binary KL bounds)**.** *Let $g_{ab} : [0,1]^2 \to [0,1]$ be given by*

$$g_{ab}(x,y) = \frac{ax+by-\min(a,b,a+b,0)}{|b|+|a|}. \tag{101}$$

Furthermore, let

$$d_{ab}^{-1}(q,c) = \sup\left\{p \in [0,1] : d\Big(g_{ab}(q,p), g_{ab}\Big(\frac{q+p}{2}, \frac{q+p}{2}\Big)\Big) \le c\right\}. \tag{102}$$

Consider the CMI setting. Then, for any a and b,

$$L_{\mathcal{D}} \le d_{ab}^{-1}\left(\hat{L}, \frac{1}{n}\sum_{i=1}^{n} I(\ell(\mathcal{A}(\widetilde{Z}_S, R), \widetilde{Z}_i); S_i|\widetilde{Z})\right). \tag{103}$$

Furthermore,

$$L_{\mathcal{D}} \le \mathbb{E}_{\widetilde{Z}}\left[d_{ab}^{-1}\left(\mathbb{E}_{R,S}\left[L_{\widetilde{Z}_S}(\mathcal{A}, \widetilde{Z}_S, R)\right], \frac{1}{n}\sum_{i=1}^{n} I^{\widetilde{Z}}(\ell(\mathcal{A}(\widetilde{Z}_S, R), \widetilde{Z}_i); S_i)\right)\right]. \tag{104}$$

Proof of Theorem 10. Fix $\tilde{z}$ and u. Let S' be a random variable with the same marginal distribution as S such that λ and S' are independent. We will use the same notation as in Corollary 2, and set $\lambda_u = \ell(\mathcal{A}(\tilde{z}_S, R), \tilde{z}_u)$, $\lambda_{S_u} = (\lambda_{u_1,S_{u_1}}, \ldots, \lambda_{u_m,S_{u_m}})$, and $\hat{\lambda}_{S_u} = \frac{1}{m}\sum_{i=1}^{m} \lambda_{u_i,S_{u_i}}$. Then,

$$\mathbb{E}_{S'}\left[\hat{\lambda}_{S'_u}\right] = \mathbb{E}_{S'}\left[\hat{\lambda}_{\bar{S}'_u}\right] = \frac{1}{m}\sum_{i=1}^{m} \frac{\lambda_{u_i,0}+\lambda_{u_i,1}}{2} = \hat{\lambda}_u. \tag{105}$$

Notice that, for any s, we have $\hat{\lambda}_u = (\hat{\lambda}_{s_u} + \hat{\lambda}_{\bar{s}_u})/2$. Since g_{ab} is linear in both of its arguments, it follows that

$$\mathbb{E}_{S'}\left[g_{ab}\Big(\hat{\lambda}_{S'_u}, \hat{\lambda}_{\bar{S}'_u}\Big)\right] = g_{ab}\Big(\hat{\lambda}_u, \hat{\lambda}_u\Big). \tag{106}$$

Thus, we can apply Lemma 2 with $\hat{\mu} = g_{ab}(\hat{\lambda}_{S'_u}, \hat{\lambda}_{\bar{S}'_u})$ and $\bar{\mu} = g_{ab}(\hat{\lambda}_u, \hat{\lambda}_u)$. Note that, since $\tilde{z}$ is fixed, the summands in $\hat{\mu}$ are independent but not identically distributed, and in particular, they do not have the same mean. This implies that [29, Eq. (17)] does not suffice and we need Lemma 2. It then follows from Corollary 2, applied with $f_\gamma(\hat{\lambda}_{S_u}, \hat{\lambda}_{\bar{S}_u}) = m d_\gamma\Big(g_{ab}\Big(\hat{\lambda}_{S_u}\Big), g_{ab}\Big(\hat{\lambda}_{\bar{S}_u}\Big)\Big)$, that

$$\sup_\gamma \mathbb{E}_{\lambda_u,S_u}\left[m d_\gamma\Big(g_{ab}\Big(\hat{\lambda}_{S_u}, \hat{\lambda}_{\bar{S}_u}\Big), g_{ab}\Big(\hat{\lambda}_u, \hat{\lambda}_u\Big)\Big)\right] \le I^{\tilde{z},u}(\lambda_u; S_u). \tag{107}$$

By Jensen's inequality, we can move the expectation inside the jointly convex function $d_\gamma(\cdot \,||\, \cdot)$ and linear function g_{ab}, and then perform the optimization over γ, to get

$$d\Big(g_{ab}\Big(\mathbb{E}_{\lambda_u,S_u}\Big[\hat{\lambda}_{S_u}\Big], \mathbb{E}_{\lambda_u,S_u}\Big[\hat{\lambda}_{\bar{S}_u}\Big]\Big), g_{ab}\Big(\mathbb{E}_{\lambda_u,S_u}\Big[\hat{\lambda}_u\Big], \mathbb{E}_{\lambda_u,S_u}\Big[\hat{\lambda}_u\Big]\Big)\Big) \le \frac{I^{\tilde{z},u}(\lambda_u; S_u)}{m}. \tag{108}$$

Finally, averaging over $\widetilde{Z}$ and U, replacing shorthands by their long forms, and again using Jensen's inequality to move the expectations inside $d(\cdot\,||\,\cdot)$ and g_{ab}, we get

$$d\left(g_{ab}\left(\hat{L}, L_{\mathcal{D}}\right)\,||\,g_{ab}\left(\frac{\hat{L}+L_{\mathcal{D}}}{2}, \frac{\hat{L}+L_{\mathcal{D}}}{2}\right)\right) \leq \frac{I(\ell(\mathcal{A}(\widetilde{Z}_S, R), \widetilde{Z}_U); S_U|\widetilde{Z}, U)}{m}. \tag{109}$$

Since the right-hand side is an increasing function of the size m of the random subset U, the tightest bound is obtained by setting $m = 1$, from which the result in (103) follows.

To prove (104), we return to (108). By averaging over U and using Jensen's inequality to move this average inside the convex function $d(\cdot\,||\,\cdot)$, we find that

$$d\Big(g_{ab}\Big(\mathbb{E}_{U,\lambda_U,S_U}\left[\hat{\lambda}_{S_u}\right]\,||\,\mathbb{E}_{U,\lambda_U,S_U}\left[\hat{\lambda}_{\bar{S}_u}\right]\Big), g_{ab}\Big(\mathbb{E}_{U,\lambda_U,S_U}\left[\hat{\lambda}_u\right], \mathbb{E}_{U,\lambda_U,S_U}\left[\hat{\lambda}_u\right]\Big)\Big) \leq \frac{I^{\tilde{z}}(\lambda_U; S_U|U)}{m}. \tag{110}$$

By the definition of d_{ab}^{-1}, this implies that

$$\mathbb{E}_{U,\lambda_U,S_U}\left[\hat{\lambda}_{\bar{S}_u}\right] \leq d_{ab}^{-1}\left(\mathbb{E}_{U,\lambda_U,S_U}\left[\hat{\lambda}_{S_u}\right], \frac{I^{\tilde{z}}(\lambda_U; S_U|U)}{m}\right). \tag{111}$$

By averaging over $\widetilde{Z}$ and replacing shorthands with their long forms, we find that

$$\mathbb{E}_{\widetilde{Z},S,R}\Big[L_{\mathcal{D}}(\mathcal{A}, \widetilde{Z}_S, R)\Big] \leq \mathbb{E}_{\widetilde{Z}}\left[d_{ab}^{-1}\left(L_{\widetilde{Z}_S}(\mathcal{A}, \widetilde{Z}_S, R), \frac{I^{\widetilde{Z}}(\ell(\mathcal{A}(\widetilde{Z}_S, R), \widetilde{Z}_U); S_U|U)}{m}\right]\right). \tag{112}$$

Since d_{ab}^{-1} is an increasing function of its second argument and $I^{\widetilde{Z}}(\ell(\mathcal{A}(\widetilde{Z}_S, R), \widetilde{Z}_U); S_U|U)/m$ is increasing in m, the tightest bound is obtained with $m = 1$. With this choice, the result in (104) follows. □

Note that we can establish (18) and (20), hence proving Theorem 4 and 5, by setting $a = 1$ and $b = 0$ in (103) and (104) respectively. However, we can also optimize over a and b, which sometimes leads to tighter bounds. As an example, $d_{0,1}^{-1}(0.3, 0.125) < d_{1,0}^{-1}(0.3, 0.125)$. This shows that $a = 1, b = 0$ does not always give the tightest result.

B.3 Single-draw bound

As mentioned in Section 3, under a technical assumption of absolute continuity, it is possible to obtain a version of Theorem 7 that holds with high probability also over the draw of R. We present this result in the following theorem.

Theorem 11 (High-probability bounds with respect to R)**.** *Let $\lambda = \ell(\mathcal{A}(\widetilde{Z}_S, R), \widetilde{Z})$. Furthermore, let $P_{\lambda|\widetilde{Z}S}$ denote the conditional distribution of λ given $\widetilde{Z}$ and S, and let $P_{\lambda|\widetilde{Z}}$ denote the conditional distribution of λ given $\widetilde{Z}$. Let $\imath(\lambda, S|\widetilde{Z}) = \log P_{\lambda|\widetilde{Z}S}/P_{\lambda|\widetilde{Z}}$ denote the conditional information density between λ and S given $\widetilde{Z}$. Assume that $P_{\lambda|\widetilde{Z}}$ is absolutely continuous with respect to $P_{\lambda|\widetilde{Z}S}$. Then, with probability at least $1-\delta$ over the draw of $\widetilde{Z}$, S, and R,*

$$L_{\widetilde{Z}_{\bar{S}}}(\mathcal{A}, \widetilde{Z}_S, R) - L_{\widetilde{Z}_S}(\mathcal{A}, \widetilde{Z}_S, R) \leq \sqrt{\frac{2}{n-1}\left(\imath(\lambda, S|\widetilde{Z}) + \log\frac{\sqrt{n}}{\delta}\right)}. \tag{113}$$

Furthermore, also with probability at least $1-\delta$ over the draw of $\widetilde{Z}$, S and R,

$$d\left(L_{\widetilde{Z}_S}(\mathcal{A}, \widetilde{Z}_S, R)\,||\,\frac{L_{\widetilde{Z}_S}(\mathcal{A}, \widetilde{Z}_S, R) + L_{\widetilde{Z}_{\bar{S}}}(\mathcal{A}, \widetilde{Z}_S, R)}{2}\right) \leq \frac{\imath(\lambda, S|\widetilde{Z}) + \log\frac{2\sqrt{n}}{\delta}}{n}. \tag{114}$$

Proof. For any function $f_\gamma(\cdot,\cdot)$, define

$$\xi_\gamma = \log \mathbb{E}_{\lambda,\widetilde{Z},S'}\left[e^{f_\gamma(\hat{\lambda}_{S'}, \hat{\lambda}_{\bar{S}'})}\right] = \log \mathbb{E}_{\lambda',\widetilde{Z},S}\left[e^{f_\gamma(\hat{\lambda}_{S'}, \hat{\lambda}_{\bar{S}'})}\right], \tag{115}$$

where we used the observation that $\lambda, \widetilde{Z}, S'$ has the same distribution as $\lambda', \widetilde{Z}, S$. By our absolute continuity assumption, [44, Prop. 17.1] implies that

$$1 = \mathbb{E}_{\lambda,\widetilde{Z},S}\left[e^{f_\gamma(\hat{\lambda}_{S'},\hat{\lambda}_{\bar{S}'})-\imath(\lambda,S|\widetilde{Z})-\xi_\gamma}\right]. \tag{116}$$

Note that if $\widetilde{Z}$ and S are fixed, the randomness of λ is fully captured by R. By Markov's inequality, we conclude that, with probability at least $1-\delta$ under the draw of $\widetilde{Z}$, S and R,

$$e^{f_\gamma(\hat{\lambda}_{S'},\hat{\lambda}_{\bar{S}'})-\imath(\lambda,S|\widetilde{Z})-\xi_\gamma} \leq \log\frac{1}{\delta} \tag{117}$$

from which it follows that

$$f_\gamma(\hat{\lambda}_{S'},\hat{\lambda}_{\bar{S}'}) \leq \log\frac{1}{\delta} + \imath(\lambda,S|\widetilde{Z}) + \xi_\gamma. \tag{118}$$

We establish the result in (113) by setting $f_\gamma(\hat{\lambda}_{S'},\hat{\lambda}_{\bar{S}'}) = \frac{(n-1)}{2}(\hat{\lambda}_{\bar{S}'} - \hat{\lambda}_{S'})^2$ and using (72). Similarly, we establish the result in (114) by setting $f_\gamma(\hat{\lambda}_{S'},\hat{\lambda}_{\bar{S}'}) = nd(\hat{\lambda}_{S'} \,||\, (\hat{\lambda}_{S'} + \hat{\lambda}_{\bar{S}'})/2)$ and using (75).

□

The bounds in Theorem 11 are given in terms of the conditional information density [34]. Assuming that the learning algorithm implements a function from a class of bounded Natarajan dimension, the conditional information density can be bounded in a similar way as was done for the e-CMI and the KL divergence in Theorem 8. We present the resulting bound in the following theorem.

Theorem 12. *Consider a multiclass classification setting, for which $\mathcal{Z} = \mathcal{X} \times \mathcal{Y}$, where $\mathcal{X}$ is the instance space and $\mathcal{Y}$ the label space, and assume that $|\mathcal{Y}| = N$. Furthermore, assume that the learning algorithm implements a function $f : \mathcal{X} \to \mathcal{Y}$ where $f \in \mathcal{F}$ belongs to a class of finite Natarajan dimension d_N [38]. Finally, assume that $2n \geq d_N + 1$. Then, with probability at least $1-\delta$ under the draw of $\widetilde{Z}$, S, and R,*

$$\imath(\lambda,S|\widetilde{Z}) \leq d_N \log\left(\binom{N}{2}\frac{2en}{d_N}\right) + \log\frac{1}{\delta}. \tag{119}$$

Proof. Note that if $\widetilde{Z}$ and S are fixed, the randomness of λ is fully captured by R. Thus, by Markov's inequality, we conclude that with probability at least $1-\delta$ under the draw of $\widetilde{Z}$, S, and R,

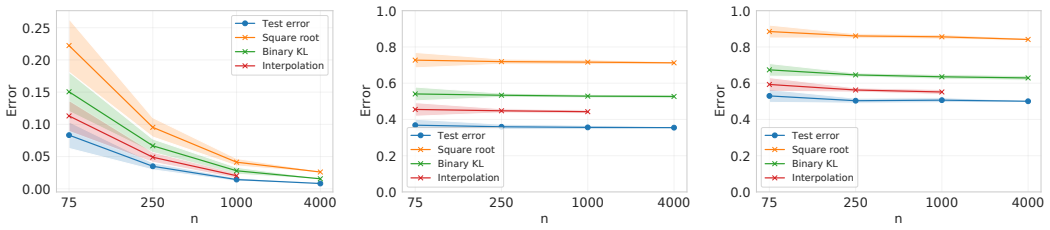
$$\imath(\lambda,S|\widetilde{Z}) = \log\frac{P_{\lambda|\widetilde{Z}S}}{P_{\lambda|\widetilde{Z}}} \leq \log\left(\frac{1}{\delta}\,\mathbb{E}_{P_{\lambda\widetilde{Z}S}}\left[\frac{P_{\lambda|\widetilde{Z}S}}{P_{\lambda|\widetilde{Z}}}\right]\right). \tag{120}$$

The right-hand side of (120) coincides with the right-hand side of (83). The desired result now follows by combining (120) and (84)-(89). □

B.4 Comparison to previous bounds

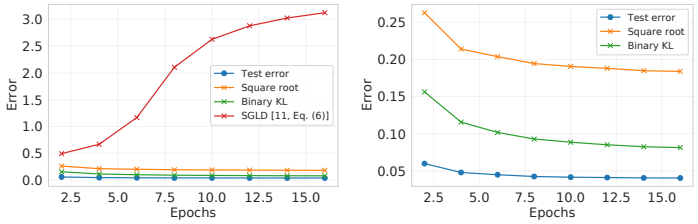
In this section, we compare the bounds in this paper to comparable results in from previous work. First, we perform a comparison with the results reported in [13], where a number of bounds that are functionally similar to ours are derived. The bounds that we derive in this paper are tighter due to the use of evaluated CMI. By the data-processing inequality for KL divergence [44, Thm. 2.2.6], our bounds can be relaxed to obtain bounds with the ordinary CMI in place of the evaluated CMI, demonstrating that they compare favorably to those of [13]. The same argument holds for the high-probability bounds.

Next, we compare (24) to the bound in [35, Corollary 1]. In terms of convergence rates, the bound in [35, Corollary 1] interpolates between our square-root and linear bounds, where the specific rate depends on the parameter β^* in the Bernstein condition in [35]. For the case of $0/1$-loss, we have that $B = 4$ and $\beta^* = 0$ in the Bernstein condition. Thus, [35, Corollary 1] has the same $1/\sqrt{n}$ rate as our square-root bound. Quantitatively, one expects our square-root bound to be tighter for several reasons: i) the bound in [35, Corollary 1] includes a constant $1/\eta_{\max} > 28.8$ that multiplies the KL divergence and $\log 1/\delta$ terms, ii) the bound in [35, Corollary 1] includes an extra $\eta_{\max}/(4n)$ term, and



(a) No label corruption (b) 50% label corruption (c) 100% label corruption

Figure 3: Numerical evaluation of the test error for the binarized MNIST setting considered in Figure 2a, but with varying degrees of label corruption, along with the upper bounds provided by the square-root bound in (4), the binary KL bound in (20) and, when applicable, the interpolation bound in (12).



(a) CIFAR10, SGLD (b) CIFAR10, SGLD (zoomed)

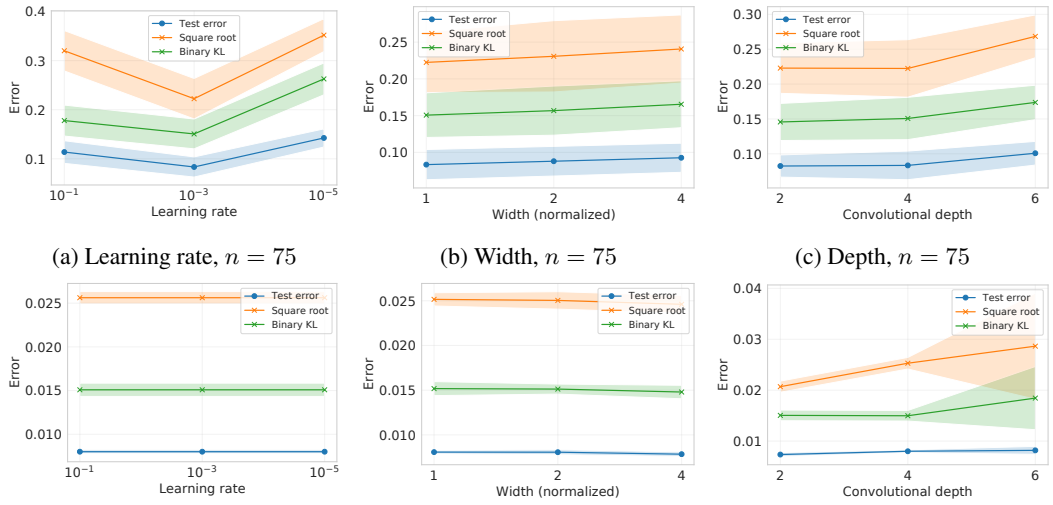
Figure 4: Numerical evaluation of the test error for a pre-trained ResNet-50 fine-tuned with SGLD on CIFAR-10, along with the upper bounds provided by the square-root bound in (4), the binary KL bound in (20), and the SGLD bound in [11, Eq. 6].

iii) the $\log 1/\delta$ term in the bound in [35, Corollary 1] appears outside of the square-root containing the KL divergence. To perform a direct quantitative comparison, some simplifying assumptions are needed. First, while the data-processing inequality implies that the KL divergence in (24) is always smaller than or equal to the KL divergence in the bound of [35, Corollary 1], we shall assume that both KL divergences equal 1. Furthermore, we set $\delta = 0.01$ and $n = 1000$. Under these assumptions, the bound in [35, Corollary 1] gives a generalization gap of approximately 2.89, which is vacuous, whereas the bound in (24) gives a generalization gap of approximately 0.13. This discrepancy arises mainly due to the large constants described above, and holds for other reasonable values of the parameters involved.

C Additional Numerical Results

In this section, we present some additional numerical results for deep learning settings.

To study a scenario with heavy overfitting, we repeat the experiment with SGD on the binarized MNIST data set, as presented in Figure 2a, but with varying degrees of label randomization. Specifically, for each sample in the binarized MNIST data set, we consider a random variable $C \sim \mathrm{Bern}(a)$, where a is the probability of corruption. If $C = 1$, the label is set to either 4 or 9, picked uniformly at random. If $C = 0$, we leave the label unchanged. For all levels of label corruption, the networks reached training errors of zero or near zero. In Figure 3a, we consider $a = 0$, so no labels are corrupted. This is the same as Figure 2a, and is included only for reference. In Figure 3b, we consider $a = 0.5$. Finally, in Figure 3c, we set $a = 1$, so that all labels are corrupted. Thus, for this scenario, the training set carries no relevant information, and the classifier completely overfits to the data set. For all levels of corruptions, the interpolation bound in (12) gives the tightest bound when applicable. Furthermore, the binary KL bound in (20) is tighter than the square-root bound in (4). The bounds give somewhat reasonable estimates of the test error. In contrast, the generalization bounds for randomized labels reported in previous works are vacuous [47, 13].



(a) Learning rate, $n = 75$ (b) Width, $n = 75$ (c) Depth, $n = 75$

(d) Learning rate, $n = 4000$ (e) Width, $n = 4000$ (f) Depth, $n = 4000$

Figure 5: Numerical evaluation of the test error for the binarized MNIST setting considered in Figure 2a, but with varying learning rate, width, and depth of the network, along with the upper bounds provided by the square-root bound in (4) and the binary KL bound in (20). For the figures in the first row, we fix $n = 75$, and for the second row, we fix $n = 4000$.

In Figure 4, we consider SGLD, as in Figure 2c, but for CIFAR10 instead of the binarized MNIST data set. Again, the binary KL bound in (20) gives the tightest result. Unlike for the binarized MNIST scenario, the SGLD bound in [11, Eq. 6] is not the tightest during early epochs.

Finally, to study the robustness of our bounds to various hyperparameter changes, we again repeat the experiment with SGD on the binarized MNIST data set, but with varying learning rate, network width, and network depth. First, we consider the case of $n = 75$, since this leads to higher test errors, making variations in it more noticeable. Second, we consider $n = 4000$ to examine whether the same qualitative conclusions hold for a larger sample size. This is shown in Figure 5. When varying the width in Figure 5b, the number of units in each of the convolutional layers of the original network, described in Table 1, is multiplied by the factor given on the horizontal axis. When varying the depth in Figure 5c, the convolutional depth of 4 corresponds to the original network, described in Table 1, the depth of 2 is the same network but with the two first convolutional layers removed, and the depth of 6 is the same network but with two additional convolutional layers with 64 units, 3×3 size, a stride of 1, and padding 1. The bounds seem to correlate well with the test error across these scenarios, and they correctly predict the values for each hyperparameter that lead to the lowest and highest test errors. This effect is noticeable for $n = 75$, where there is significant variation between the different hyperparameter values. For $n = 4000$, this variation is heavily reduced, but the overall behavior of our bounds is still consistent with the behavior of the test error.

D Experimental Details

In this section, we describe the training procedures, network architectures, and experimental details used in Section 6. Note that the setups are the same as those considered in [17]. The experiments were run on Google Colab Pro GPUs.

In all experiments, we estimate the test error of the networks and the upper bounds provided by the square-root bound in (4) and the binary KL bound in (20) (and [11, Eq. (6)] for Figure 2c) by drawing k_1 samples of $\tilde{Z}$, which consists of n pairs of samples drawn randomly from the corresponding dataset, and k_2 samples of S (and R for Figure 2c). We run the training algorithm for each of these samples, compute the training loss, and estimate the population loss using $\tilde{z}_s$. For each $\tilde{z}$, we estimate the mutual information $I^{\tilde{z}}(\ell(\mathcal{A}(\tilde{z}_S, R), \tilde{z}_i); S_i)$ using a plug-in estimator [53]. Based on these estimates, the bounds are computed. The results in Figure 2 illustrate the estimated averages, with shaded areas indicating one standard deviation.

Table 1: The neural network used for the binarized MNIST experiments in Figure 2a and Figure 2c.

CONV. LAYER, 32 UNITS, 4×4 SIZE, STRIDE 2, PADDING 1, BATCH NORM., RELU ACTIVATION
CONV. LAYER, 32 UNITS, 4×4 SIZE, STRIDE 2, PADDING 1, BATCH NORM., RELU ACTIVATION
CONV. LAYER, 64 UNITS, 3×3 SIZE, STRIDE 2, PADDING 0, BATCH NORM., RELU ACTIVATION
CONV. LAYER, 256 UNITS, 3×3 SIZE, STRIDE 1, PADDING 0, BATCH NORM., RELU ACTIVATION
FULLY CONNECTED LAYER, 128 UNITS, RELU ACTIVATION
FULLY CONNECTED LAYER, 2 UNITS, LINEAR ACTIVATION

D.1 Binarized MNIST

For Figure 2a and 2c, we consider the network described in Table 1. The dataset that we use consist of the parts of MNIST that corresponds to the digits 4 and 9. Both Figure 2a and Figure 2c are based on 5 samples of $\widetilde{Z}$, with 30 samples of S for each $\tilde{z}$.

D.1.1 Adam

For Figure 2a, we optimize the network using the Adam algorithm, with a 0.001 learning rate and $\beta_1 = 0.9$, for 200 epochs with a batch size of 128.

D.1.2 SGLD

For Figure 2c, we optimize the network using SGLD for 40 epochs with a batch size of 100. The learning rate starts at 0.01 and decays by a factor of 0.9 after each 100 iterations. The inverse temperature schedule is given by $\min(4000, \max(100, 10e^{t/100}))$ where t is the iteration.

D.2 CIFAR10 and SGD

For Figure 2b, we consider the network ResNet-50, which is pretrained on Imagenet. Then, we fine-tune it on CIFAR10 using SGD with a 0.01 learning rate and 0.9 momentum for 40 epochs with a batch size of 64. During training, we use random horizontal flips and random 28×28 cropping as data augmentations. The values in the figure are based on 2 samples of $\widetilde{Z}$, with 40 samples of S for each $\tilde{z}$.

References

[1] J. Shawe-Taylor and R. C. Williamson. A PAC analysis of a Bayesian estimator. In *Proc. Conf. Learn. Theory (COLT)*, July 1997.

[2] D. A. McAllester. Some PAC-Bayesian theorems. In *Proc. Conf. Learn. Theory (COLT)*, Madison, WI, USA, July 1998.

[3] B. Guedj. A primer on PAC-Bayesian learning. *arXiv*, Jan. 2019.

[4] P. Alquier. User-friendly introduction to PAC-Bayes bounds. *arXiv*, Nov. 2021.

[5] D. Russo and J. Zou. Controlling bias in adaptive data analysis using information theory. In *Proc. Artif. Intell. Statist. (AISTATS)*, Cadiz, Spain, May 2016.

[6] A. Xu and M. Raginsky. Information-theoretic analysis of generalization capability of learning algorithms. In *Proc. Conf. Neural Inf. Process. Syst. (NeurIPS)*, Long Beach, CA, USA, Dec. 2017.

[7] A. R. Asadi, E. Abbe, and S. Verdú. Chaining mutual information and tightening generalization bounds. In *Proc. Conf. Neural Inf. Process. Syst. (NeurIPS)*, Montreal, Canada, Dec. 2018.

[8] H. Hafez-Kolahi, Z. Golgooni, S. Kasaei, and M. Soleymani. Conditioning and processing: Techniques to improve information-theoretic generalization bounds. In *Proc. Conf. Neural Inf. Process. Syst. (NeurIPS)*, Vancouver, Canada, Dec. 2020.

[9] B. Rodríguez-Gálvez, G. Bassi, R. Thobaben, and M. Skoglund. On random subset generalization error bounds and the stochastic gradient Langevin dynamics algorithm. In *Proc. Inf. Theory Workshop (ITW)*, Riva del Garda, Italy, Apr. 2020.

[10] Y. Bu, S. Zou, and V. V. Veeravalli. Tightening mutual information-based bounds on generalization error. *IEEE J. Sel. Areas Inf. Theory*, 1(1):121–130, May 2020.

[11] J. Negrea, M. Haghifam, G. K. Dziugaite, A. Khisti, and D. M. Roy. Information-theoretic generalization bounds for SGLD via data-dependent estimates. In *Proc. Conf. Neural Inf. Process. Syst. (NeurIPS)*, Vancouver, Canada, Dec. 2019.

[12] M. Haghifam, J. Negrea, A. Khisti, D.M. Roy, and G.K. Dziugaite. Sharpened generalization bounds based on conditional mutual information and an application to noisy, iterative algorithms. In *Proc. Conf. Neural Inf. Process. Syst. (NeurIPS)*, Vancouver, Canada, 12 2020.

[13] F. Hellström and G. Durisi. Fast-rate loss bounds via conditional information measures with applications to neural networks. In *Proc. IEEE Int. Symp. Inf. Theory (ISIT)*, Melbourne, Australia, July 2021.

[14] R. Zhou, C. Tian, and T. Liu. Individually conditional individual mutual information bound on generalization error. In *Proc. IEEE Int. Symp. Inf. Theory (ISIT)*, Melbourne, Australia, July 2021.

[15] G. Neu, G. K. Dziugiate, M. Haghifam, and D. M.. Roy. Information-theoretic generalization bounds for stochastic gradient descent. In *Proc. Conf. Learn. Theory (COLT)*, Boulder, CO, USA, Aug. 2021.

[16] T. Steinke and L. Zakynthinou. Reasoning about generalization via conditional mutual information. In *Proc. Conf. Learn. Theory (COLT)*, Graz, Austria, July 2020.

[17] H. Harutyunyan, M. Raginsky, G. Ver Steeg, and A. Galstyan. Information-theoretic generalization bounds for black-box learning algorithms. In *Proc. Conf. Neural Inf. Process. Syst. (NeurIPS)*, Virtual Conference, Dec. 2021.

[18] F. Hellström and G. Durisi. Data-dependent PAC-Bayesian bounds in the random-subset setting with applications to neural networks. In *Workshop on Inf.-Theoretic Methods Rigorous, Responsible, and Reliable Mach. Learn. (ITR3)*, Virtual conference, July 2021.

[19] J. Langford and M. Seeger. Bounds for averaging classifiers. *CMU Technical report*, CMU-CS-01-102, 2001.

[20] M. Seeger. PAC-Bayesian generalisation error bounds for Gaussian process classification. *J. of Mach. Learn. Res.*, 3:233–269, Oct. 2002.

[21] J. Langford. *Quantitatively Tight Sample Complexity Bounds*. PhD thesis, Carnegie Mellon University, Pittsburgh, PA, USA, 2002.

[22] A. Maurer. A note on the PAC Bayesian theorem. *arXiv*, Nov. 2004.

[23] P. Germain, A. Lacasse, F. Laviolette, and M. Marchand. PAC-Bayesian learning of linear classifiers. In *Proc. Int. Conf. Mach. Learning (ICML)*, Montreal, Canada, June 2009.

[24] L. Bégin, P. Germain, F. Laviolette, and J. F. Roy. PAC-Bayesian theory for transductive learning. In *Proc. Int. Conf. Artif. Intell. Statist. (AISTATS)*, Reykjavik, Iceland, Apr. 2014.

[25] O. Rivasplata, I. Kuzborskij, C. Szepesvari, and J. Shawe-Taylor. PAC-Bayes analysis beyond the usual bounds. In *Proc. Conf. Neural Inf. Process. Syst. (NeurIPS)*, Vancouver, Canada, Dec. 2020.

[26] M. Haghifam, G. K. Dziugaite, S. Moran, and D. M. Roy. Towards a unified information-theoretic framework for generalization. In *Proc. Conf. Neural Inf. Process. Syst. (NeurIPS)*, Virtual Conference, Dec. 2021.

[27] O. Catoni. *PAC-Bayesian Supervised Classification: The Thermodynamics of Statistical Learning*, volume 56. IMS Lecture Notes Monogr. Ser., 2007.

[28] M. Haddouche, B. Guedj, O. Rivasplata, and J. Shawe-Taylor. PAC-Bayes unleashed: Generalisation bounds with unbounded losses. *Entropy*, 23(10), Oct. 2021.

[29] D. A. McAllester. A PAC-Bayesian tutorial with a dropout bound. *arXiv*, July 2013.

[30] Y. Seldin, F. Laviolette, N. Cesa-Bianchi, J. Shawe-Taylor, and P. Auer. PAC-Bayesian inequalities for martingales. *IEEE Trans. Inf. Theory*, 58(12):7086–7093, Aug. 2012.

[31] W. Hoeffding. On the distribution of the number of successes in independent trials. *The Annals of Mathematical Statistics*, 27(3):713–721, Sep. 1956.

[32] J. Guan, Z. Lu, and Y. Liu. Improved generalization risk bounds for meta-learning with PAC-Bayes-kl analysis. *https://openreview.net/forum?id=XgS9YPYtdj*, 2021.

[33] Z. Mhammedi, P. Grünwald, and B. Guedj. PAC-Bayes un-expected Bernstein inequality. In *Proc. Conf. Neural Inf. Process. Syst. (NeurIPS)*, Vancouver, Canada, Dec. 2019.

[34] F. Hellström and G. Durisi. Generalization bounds via information density and conditional information density. *IEEE J. Sel. Areas Inf. Theory*, 1(3):824–839, Dec. 2020.

[35] P. Grünwald, T. Steinke, and L. Zakynthinou. PAC-Bayes, MAC-Bayes and conditional mutual information: Fast rate bounds that handle general VC classes. In *Proc. Conf. Learn. Theory (COLT)*, Boulder, CO, USA, Aug. 2021.

[36] Hrayr Harutyunyan, Greg Ver Steeg, and Aram Galstyan. Formal limitations of sample-wise information-theoretic generalization bounds. In *2022 IEEE Inf. Theory Workshop (ITW)*, Mumbai, India, Nov. 2022.

[37] H. Wang, Y. Huang, R. Gao, and F. Calmon. Analyzing the generalization capability of SGLD using properties of Gaussian channels. In *Proc. Conf. Neural Inf. Process. Syst. (NeurIPS)*, Virtual Conference, Dec. 2021.

[38] B. K. Natarajan. On learning sets and functions. *Machine Learning*, 4:67–97, 1989.

[39] Y. Guermeur. Large margin multi-category discriminant models and scale-sensitive psi-dimensions. Research report, INRIA, 2004.

[40] S. Shalev-Shwartz and S. Ben-David. *Understanding Machine Learning: From Theory to Algorithms*. Cambridge Univ. Press, Cambridge, U.K., 2014.

[41] L. Deng. The MNIST database of handwritten digit images for machine learning research. *IEEE Signal Process. Mag.*, 29(6):141–142, 2012.

[42] A. Krizhevsky. Learning multiple layers of features from tiny images. Technical report, 2009.

[43] M. D. Donsker and S. R. S. Varadhan. Asymptotic evaluation of certain Markov process expectations for large time, i. *Comm. Pure Appl. Math*, 28(1):1–47, Jan. 1975.

[44] Y. Polyanskiy and Y. Wu. *Lecture Notes On Information Theory*. 2019.

[45] M. J. Wainwright. *High-Dimensional Statistics: a Non-Asymptotic Viewpoint*. Cambridge Univ. Press, Cambridge, U.K., 2019.

[46] D. Haussler and P. M. Long. A generalization of Sauer's lemma. *J. Combinatorial Theory, Series A*, 71(2):219–240, 1995.

[47] G. K. Dziugaite and D. M. Roy. Computing nonvacuous generalization bounds for deep (stochastic) neural networks with many more parameters than training data. In *Proc. Conf. Uncertainty in Artif. Intell. (UAI)*, Sydney, Australia, Aug. 2017.

[48] I. Csiszar and J. Körner. *Information Theory: Coding Theorems for Discrete Memoryless Systems*. Cambridge Univ. Press, Cambridge, U.K., 2nd edition, 2011.

[49] G. K. Dziugaite and D. M. Roy. Data-dependent PAC-Bayes priors via differential privacy. In *Proc. Conf. Neural Inf. Process. Syst. (NeurIPS)*, Montreal, Canada, Dec. 2018.

[50] A. Ambroladze, E. Parrado-Hernandez, and J. Shawe-Taylor. Tighter PAC-Bayes bounds. In *Proc. Conf. Neural Inf. Process. Syst. (NeurIPS)*, Vancouver, Canada, Dec. 2006.

[51] G.K. Dziugaite, K. Hsu, W. Gharbieh, and D.M. Roy. On the role of data in PAC-Bayes bounds. In *Proc. Artif. Intell. Statist. (AISTATS)*, San Diego, CA, USA, Apr. 2021.

[52] M. Perez-Ortiz, O. Risvaplata, J. Shawe-Taylor, and C. Szepesvari. Tighter risk certificates for neural networks. *J. of Mach. Learn. Res.*, 22(227), Aug. 2021.

[53] L. Paninski. Estimation of entropy and mutual information. *Neural Computation*, 15(6):1191–1253, June 2003.