702 A APPENDIX

704 A.1 PROOFS IN SEC. 2

Lemma A.1 (Equivalence condition). If we assume (1) identical ground truth labeling function in the training and deployment g = g', (2) Restricted TV distance between training and deployment $TV(P_x, Q_x) \le \kappa$, then with probability $1 - 2\epsilon - \kappa$, PDD is equivalent to D-PDD.

Proof. Step 1: Def 1 \rightarrow Def 2. If g' = g, it is clear

$$\operatorname{err}(f, \boldsymbol{Q}_g) > \operatorname{err}(f, \boldsymbol{P}_g)$$

Then we set $h = g \in \mathcal{H}$, we have Def 2.

Step 2: Def 2 \rightarrow Def 1. If g' = g, we need to prove

$$\operatorname{err}(f, \boldsymbol{Q}_g) > \operatorname{err}(f, \boldsymbol{P}_g)$$

717 Given the disagreement condition in Def 2,

$$\operatorname{err}(f, \boldsymbol{Q}_h) > \operatorname{err}(f, \boldsymbol{P}_h)$$

We need to demonstrate h = g with high probability, given the binary risk definition and Markov inequality, we have high probability $1 - \epsilon$ such that:

$$h = g, \quad f = g$$

Therefore $\operatorname{err}(f, P_g) = \operatorname{err}(f, P_h)$ happens in probability P with $1 - \epsilon$. Then we consider this events in Q, given a small TV-distance (κ) between P and Q, we have

$$|\boldsymbol{P}(f(x) = g(x)) - \boldsymbol{Q}(f(x) = g(x))| \le \mathrm{TV}(\boldsymbol{P}_x, \boldsymbol{Q}_x) \le \kappa$$

Thus with high probability $1 - \kappa - \epsilon$ in Q, we still have f(x) = g(x). Union bounding yields the desired conclusion.

730 A.2 PROOFS IN SEC. 4

Lemma A.2. For any $\gamma > 0$, $\mu > \epsilon_q$, we have $\widehat{\operatorname{err}}(h; Q_f) \le \mu$ for all $h \in \mathcal{H}_p$ with probability at *least* $1 - \gamma$ *if*

$$m \in \mathcal{O}\left(\frac{d_p + \ln\frac{1}{\gamma}}{\left(\mu - \epsilon_q\right)^2}\right) \tag{14}$$

Proof. We use the generalization bound for agnostic learning in Shalev-Shwartz & Ben-David (2014).

$$ce^{d_p}e^{-\epsilon^2 m} \ge \Pr_{X,Y \sim \boldsymbol{Q}_{1-f}^m} \left[\exists h \in \mathcal{H}_p : \operatorname{err}(h; \boldsymbol{Q}_{1-f}) - \widehat{\operatorname{err}}(h; \boldsymbol{Q}_{1-f}) \ge \epsilon\right]$$
(15)

$$= \Pr_{X, Y \sim \boldsymbol{Q}_{1-f}^{m}} \left[\exists h \in \mathcal{H}_{p} : \widehat{\operatorname{err}}(h; \boldsymbol{Q}_{f}) \ge \operatorname{err}(h; \boldsymbol{Q}_{f}) + \epsilon \right]$$
(16)

$$\geq \Pr_{X, Y \sim \boldsymbol{Q}_{1-f}^{m}} \left[\exists h \in \mathcal{H}_{p} : \widehat{\operatorname{err}}(h; \boldsymbol{Q}_{f}) \geq \epsilon_{q} + \epsilon \right]$$
(17)

747 Choose $\epsilon = \mu - \epsilon_q$ for any $\mu > \epsilon_q$. Now,

$$ce^{d_p}e^{-\epsilon^2 m} \le \gamma \tag{18}$$

$$m \in \mathcal{O}\left(\frac{d_p + \ln\frac{1}{\gamma}}{\left(\mu - \epsilon_q\right)^2}\right) \tag{19}$$

Lemma A.3. For any $h \in \mathcal{H}$, if the $\widehat{\operatorname{err}}(h; P_f) \leq \epsilon_f - \epsilon_0$ then with probability at least $1 - \mathcal{O}(\exp(-n\epsilon_0^2 + d))$, h will be in \mathcal{H}_p

Proof. We use the generalization bound for agnostic learning in Shalev-Shwartz & Ben-David (2014).

$$ce^{d}e^{-\epsilon^{2}n} \ge \Pr_{X,Y\sim P_{g}^{n}}\left[\exists h \in \mathcal{H} : \operatorname{err}(h; P_{g}) - \widehat{\operatorname{err}}(h; P_{g}) \ge \epsilon\right]$$
 (20)

$$= \Pr_{X, Y \sim \boldsymbol{P}_{g}^{n}} \left[\exists h \in \mathcal{H} : \operatorname{err}(h; \boldsymbol{P}_{g}) \ge \widehat{\operatorname{err}}(h; \boldsymbol{P}_{g}) + \epsilon \right]$$
(21)

$$\geq \Pr_{X,Y \sim \boldsymbol{P}_g^n} \left[\exists h \in \mathcal{H} : \operatorname{err}(h; \boldsymbol{P}_g) \geq \epsilon_f - \epsilon_0 + \epsilon \right]$$
(22)

Choose $\epsilon = \epsilon_0$ to get

$$\Pr_{X,Y \sim \boldsymbol{P}_g^n} \left[\exists h \in \mathcal{H} : \operatorname{err}(h; \boldsymbol{P}_g) \ge \epsilon_f \right] \le c e^d e^{-\epsilon^2 n}$$
(23)

Theorem A.4. For $\gamma \leq \alpha$, when there is no deteriorating shift, for a chosen significance level of α , the FPR of Algo. 2 is at most $\gamma + (1 - \gamma) \mathcal{O} \left(\exp \left(-n\epsilon_0^2 + d \right) \right)$ if

$$m \in \mathcal{O}\left(\left(\frac{1-\sqrt{\delta}}{\epsilon_p - \epsilon_q}\right)^2 \left(d_p + \ln\frac{1}{\gamma}\right)\right)$$
(24)

and
$$\epsilon_p - \epsilon_q > 0$$
, where $\delta = \frac{d_p + \ln \frac{1}{\alpha}}{d_p + \ln \frac{1}{\gamma}}$

Proof. We show that in the case of no deteriorating shift (which implies $\epsilon_p \ge \epsilon_q$) the false positive rate cannot be more than α and also having more samples from Q_x will decrease the false positive rate if $\epsilon_p > \epsilon_q$.

We assume that during pre-training phase, while populating Φ we discard disagreement from $h \notin \mathcal{H}_p$ i.e., not satisfying the constraint $\operatorname{err}(h; P_f) \leq \epsilon_f$. We cannot do the same during the detection phase since the detection phase is time-sensitive. Due to this, we have to account for $h \notin \mathcal{H}_p$ in the FPR calculation.

Now, FPR can be written and bounded as follows. Let μ be the disagreement at $1 - \alpha$ percentile of Φ

$$FPR = \Pr\left[\widehat{err}(h; \boldsymbol{Q}_f) \ge \mu\right]$$
(25)

$$= \Pr\left[\left\{\left\{h \notin \mathcal{H}_p\right\} \land \left\{\widehat{\operatorname{err}}(h; \boldsymbol{Q}_f) \ge \mu\right\}\right\} \lor \left\{\left\{h \in \mathcal{H}_p\right\} \land \left\{\widehat{\operatorname{err}}(h; \boldsymbol{Q}_f) \ge \mu\right\}\right\}\right]$$
(26)

$$\leq \Pr\left[\{h \notin \mathcal{H}_p\} \lor \{\{h \in \mathcal{H}_p\} \land \{\widehat{\operatorname{err}}(h; \boldsymbol{Q}_f) \ge \mu\}\}\right]$$
(27)

$$\leq \Pr\left[h \notin \mathcal{H}_p\right] + \Pr\left[\left\{\widehat{\operatorname{err}}(h; \boldsymbol{Q}_f) \geq \mu\right\} \mid \{h \in \mathcal{H}_p\}\right] \Pr\left[h \in \mathcal{H}_p\right]$$
(28)

$$= \gamma + (1 - \gamma) \Pr\left[h \notin \mathcal{H}_p\right]$$
⁽²⁹⁾

$$FPR \le \gamma + (1 - \gamma) \mathcal{O}\left(\exp\left(-n\epsilon_0^2 + d\right)\right)$$
(30)

where last equation comes from A.3 and $\gamma := \Pr \left[\{ \widehat{\operatorname{err}}(h; \boldsymbol{Q}_f) \ge \mu \} \mid \{h \in \mathcal{H}_p\} \right]$

Now, we derive sample complexity m in terms of γ . Using A.2 on P with $1 - \alpha$ probability we get

$$m \in \mathcal{O}\left(\frac{d_p + \ln\frac{1}{\alpha}}{\left(\mu - \epsilon_p\right)^2}\right) \tag{31}$$

We use
$$\mu \in \Omega\left(\epsilon_p + \sqrt{\frac{d_p + \ln \frac{1}{\alpha}}{m}}\right)$$
 from above while using A.2 on \boldsymbol{Q} with $1 - \gamma$ probability to get

$$m \in \mathcal{O}\left(\left(\frac{1-\sqrt{\frac{d_p+\ln\frac{1}{\alpha}}{d_p+\ln\frac{1}{\gamma}}}}{(\epsilon_p-\epsilon_q)}\right)^2 \left(d_p+\ln\frac{1}{\gamma}\right)\right) \quad \text{for } \gamma < \alpha \tag{32}$$

Note that since the chosen μ was greater than ϵ_p and we are dealing with the case $\epsilon_p > \epsilon_q$, we get that the chosen μ is greater than ϵ_q . Thus the requirement of μ is satisfied for A.2 while using for Q.

This theorem shows that when there are non deteriorating shifts (specifically $\epsilon_p > \epsilon_q$) FPR may be even less than α , given m and n is sufficiently large. The more samples from Q_x we have the lesser the FPR in these cases. For any general case, by setting $\gamma = \alpha$ (i.e., $\delta = 1$) in the above theorem, we obtain the following:

816
Corollary A.5. For a chosen significance level α , the FPR of the P-PDDM algorithm is no more than $\alpha + (1 - \alpha) \mathcal{O}(\exp(-n\epsilon_0^2 + d)).$

817 Note that this statement is independent of m and the distribution shift. If n is sufficiently large, the 818 exponential term is small. This is often the case when the base classifier error ϵ_f is small, which is an 819 indicator that a large number of samples (n) were available from P_g . Ignoring non deteriorating shift 820 (and $Q_x \neq P_x$) cases while calculating Φ in Algo. 2 does not adversely affect the FPR of the test.

Lemma A.6. For any $\beta > 0, \mu < \epsilon_q$, there exists an $h \in \mathcal{H}_p$ such that $\widehat{\operatorname{err}}(h; Q_f) \ge \mu$ with probability at least $1 - \beta$ if

$$m \ge \mathcal{O}\left(\frac{d_q + \ln\frac{1}{\beta}}{(\epsilon_q - \mu)^2}\right)$$
(33)

Proof. We use the generalization bound for agnostic learning case Shalev-Shwartz & Ben-David (2014).

$$ce^{d_p}e^{-\epsilon^2 m} \ge \Pr_{X,Y \sim \boldsymbol{Q}_{1-f}^m} \left[\exists h \in \mathcal{H}_p : \widehat{\operatorname{err}}(h; \boldsymbol{Q}_{1-f}) - \operatorname{err}(h; \boldsymbol{Q}_{1-f}) \ge \epsilon \right]$$
(34)

$$= \Pr_{X, Y \sim \boldsymbol{Q}_{1-f}^{m}} \left[\exists h \in \mathcal{H}_{p} : \widehat{\operatorname{err}}(h; \boldsymbol{Q}_{f}) \le \operatorname{err}(h; \boldsymbol{Q}_{f}) - \epsilon \right]$$
(35)

$$\stackrel{(a)}{=} \Pr_{X,Y \sim \boldsymbol{Q}_{1-f}^{m}} \left[\forall h \in \mathcal{H}_{p} : \widehat{\operatorname{err}}(h; \boldsymbol{Q}_{f}) \leq \epsilon_{q} - \epsilon \right]$$
(36)

where (a) follows from Def. 4

838 Choose $\epsilon = \epsilon_q - \mu$ for any $\mu < \epsilon_q$

$$ce^{d_q}e^{-\epsilon^2 m} \le \beta \tag{37}$$

$$m \ge \mathcal{O}\left(\frac{d_q + \ln\frac{1}{\beta}}{(\epsilon_q - \mu)^2}\right)$$
(38)

Proposition A.7 (D-PDD and TV distance). *The relations between* ξ (*in Def.* 5), η (*in Def.* 6), and ϵ_p , ϵ_q (*in Def.* 3 and 4) are as follows:

$$\xi = \mathrm{TV} - 2\eta \ge 0 \tag{39}$$

$$\xi \ge \epsilon_q - \epsilon_p \ge \xi - 2\epsilon_f \tag{40}$$

Proof. Recall the definition of U from 6. We first derive the Bayes error in terms of TV distance. Let

$$A = \{ x \in \mathcal{X} \mid \boldsymbol{Q}_x(x) \le \boldsymbol{P}_x(x) \}$$

$$\tag{41}$$

$$A' = \{x \in \mathcal{X} \mid \boldsymbol{Q}_x(x) > \boldsymbol{P}_x(x)\}$$

$$(42)$$

The TV distance is equal to half of the L_1 distance. Note that $P_x(A) + P_x(A') = 1$ and similarly for Q_x .²

$$TV(\boldsymbol{P}_x, \boldsymbol{Q}_x) = \frac{1}{2} \left(\boldsymbol{P}_x(A) - \boldsymbol{Q}_x(A) + \boldsymbol{Q}_x(A') - \boldsymbol{P}_x(A') \right)$$
(43)

$$=1-\boldsymbol{P}_{x}(A')-\boldsymbol{Q}_{x}(A) \tag{44}$$

²With some abuse of notation, we use the same notation for both pdf and probability measure.

Now, we use the definition of U and the above TV relation to get the following Now, we use the definition of U and the above TV relation to get the following

$$\operatorname{err}\left(f_{\text{bayes}};\boldsymbol{U}\right) = \frac{1}{2}\left(\operatorname{err}\left(f_{\text{bayes}};\boldsymbol{P}_{f}\right) + \operatorname{err}\left(f_{\text{bayes}};\boldsymbol{Q}_{1-f}\right)\right) = \frac{1}{2}\left(\boldsymbol{Q}_{x}(A) + \boldsymbol{P}_{x}(A')\right) \quad (45)$$

$$= \frac{1}{2} \left(1 - \mathrm{TV}(\boldsymbol{P}_x, \boldsymbol{Q}_x) \right) \tag{46}$$

Next, with the above result and η in Eq. 6 we derive Eq. 8

=

$$\eta + \operatorname{err}(f_{\text{bayes}}; \boldsymbol{U}) = \min_{h \in \mathcal{H}_p} \operatorname{err}(h; \boldsymbol{U}) = \frac{1}{2} \min_{h \in \mathcal{H}_p} \left(\operatorname{err}(h; \boldsymbol{P}_f) + \operatorname{err}(h; \boldsymbol{Q}_{1-f}) \right)$$
(47)

$$2\eta + 1 - \mathrm{TV} = \min_{h \in \mathcal{H}_p} \left(\operatorname{err}(h; \boldsymbol{P}_f) + \operatorname{err}(h; \boldsymbol{Q}_{1-f}) \right) \ge \min_{h \in \mathcal{H}_p} \operatorname{err}(h; \boldsymbol{Q}_{1-f})$$
(48)

$$2\eta + 1 - \mathrm{TV} = \min_{h \in \mathcal{H}_p} \left(\operatorname{err}(h; \boldsymbol{P}_f) - \operatorname{err}(h; \boldsymbol{Q}_f) \right) + 1$$
(49)

$$2\eta - \mathrm{TV} = \min_{h \in \mathcal{H}_p} - (\mathrm{err}(h; \boldsymbol{Q}_f) - \mathrm{err}(h; \boldsymbol{P}_f))$$
(50)

$$TV - 2\eta = \max_{h \in \mathcal{H}_p} \left(\operatorname{err}(h; \boldsymbol{Q}_f) - \operatorname{err}(h; \boldsymbol{P}_f) \right) = \xi$$
(51)

For Eq. 9, we use Eq. 48 and the above result to get the following

$$\epsilon_q = \max_{h \in \mathcal{H}_p} \operatorname{err}(h; \boldsymbol{Q}_f) = 1 - \min_{h \in \mathcal{H}_p} \operatorname{err}(h; \boldsymbol{Q}_{1-f}) \ge \operatorname{TV} - 2\eta = \xi$$
(52)

We can write an inequality for errors similar to triangle inequality as follows

$$\operatorname{err}(h; \boldsymbol{P}_f) \le \operatorname{err}(h; \boldsymbol{P}_g) + \operatorname{err}(g; \boldsymbol{P}_f)$$
(53)

$$= \operatorname{err}(h; \boldsymbol{P}_g) + \operatorname{err}(f; \boldsymbol{P}_g) = \operatorname{err}(h; \boldsymbol{P}_g) + \epsilon_f$$

$$\epsilon_p = \max_{h \in \mathcal{H}_p} \operatorname{err}(h; \boldsymbol{P}_f) \le \max_{h \in \mathcal{H}_p} \operatorname{err}(h; \boldsymbol{P}_g) + \epsilon_f = 2\epsilon_f$$
(55)

The last equality follows from the definition of \mathcal{H}_p . Thus we get

$$\epsilon_q - \epsilon_p \ge \xi - 2\epsilon_f \tag{56}$$

(54)

By definition it follows that $\xi \ge \epsilon_q - \epsilon_p$

Proposition A.8. For $\beta > 0$, when the deteriorating shift occurs, for a chosen significance level of α , the TPR of Algo. 2 is at least $(1 - \beta) (1 - \mathcal{O} (\exp (-n\epsilon_0^2 + d)))$ if

$$m \in \mathcal{O}\left(\left(\frac{1+\sqrt{\delta}}{\xi-2\epsilon_f}\right)^2 \left(d_p + \ln\frac{1}{\beta}\right)\right)$$
(57)

and $\epsilon_q - \epsilon_p > 0$, where $\delta = \frac{d_p + \ln \frac{1}{\alpha}}{d_p + \ln \frac{1}{\beta}}$

Proof. Similar to the proof of Theorem. 4.2, we derive the statistical power (TPR) of the test as follows. Let μ be the disagreement at $1 - \alpha$ percentile of Φ

$$TPR = 1 - \Pr\left[\widehat{err}(h; \boldsymbol{Q}_f) \le \mu\right]$$
(58)

$$= 1 - \Pr\left[\left\{\left\{h \notin \mathcal{H}_p\right\} \land \left\{\widehat{\operatorname{err}}(h; \boldsymbol{Q}_f) \le \mu\right\}\right\} \lor \left\{\left\{h \in \mathcal{H}_p\right\} \land \left\{\widehat{\operatorname{err}}(h; \boldsymbol{Q}_f) \le \mu\right\}\right\}\right]$$
(59)

$$\geq 1 - \Pr\left[\{h \notin \mathcal{H}_p\} \lor \{\{h \in \mathcal{H}_p\} \land \{\widehat{\operatorname{err}}(h; \boldsymbol{Q}_f) \leq \mu\}\}\right]$$
(60)

$$\geq 1 - \Pr\left[h \notin \mathcal{H}_p\right] - \Pr\left[\left\{\widehat{\operatorname{err}}(h; \boldsymbol{Q}_f) \leq \mu\right\} | \left\{h \in \mathcal{H}_p\right\}\right] \Pr\left[h \in \mathcal{H}_p\right]$$
(61)

$$= (1 - \beta) \Pr [h \in \mathcal{H}_p]$$

$$TPR \in (1 - \beta) \left(1 - \mathcal{O}\left(\exp\left(-n\epsilon_0^2 + d\right)\right)\right)$$
(62)
(63)

where last equation comes from A.3 and $\beta := \Pr\left[\{\widehat{\operatorname{err}}(h; \boldsymbol{Q}_f) \leq \mu\} \mid \{h \in \mathcal{H}_p\}\right]$

915 Next, we derive the sample complexity m in terms of β . We show that there exists a μ^* such that 916 both A.2 (for P and α) and A.6 (for Q and β) hold.

$$\epsilon_p < \mu < \epsilon_q \tag{64}$$

This implies some μ exists if $\epsilon_q - \epsilon_p > 0$

We find optimal μ^* such that the maximum of m in Eq. 14 and Eq. 33 is minimized.

$$\left(\frac{\mu - \epsilon_p}{\epsilon_q - \mu}\right)^2 = \frac{d_p + \ln\frac{1}{\alpha}}{d_p + \ln\frac{1}{\beta}} := \delta$$
(65)

$$\mu^* = \frac{\epsilon_p + \sqrt{\delta}\epsilon_q}{1 + \sqrt{\delta}} \tag{66}$$

Plugging this μ^* in Eq. 33 gives

$$m \in \mathcal{O}\left(\frac{d+\ln\frac{1}{\beta}}{\left(\epsilon_q - \epsilon_p\right)^2} \left(1 + \sqrt{\frac{d+\ln\frac{1}{\alpha}}{d+\ln\frac{1}{\beta}}}\right)^2\right)$$
(67)

931 Use Eq. 9 to get the result.932

 ξ in the denominator indicates that as the shift becomes more deteriorating, it is easier (fewer samples m) to monitor, indicating the effectiveness of the D-PDDM algorithm. Also, having a high-quality base classifier (low ϵ_f) is better for D-PDDM which was also seen in Eq. 9 where low ϵ_f makes the algorithm more faithful. Note that m depends on d_p which can be much less than d which n depends on, suggesting that monitoring may be effective in few-shot settings. The dependence on n is due to the requirement of satisfaction of condition 1 in Def. 2. In the optimization problems in Algo. 1, the empirical constraint is satisfied but the population constraint will be satisfied either for larger ϵ_0 or for sufficiently large n as seen in the theorem.

941 Next, we move to the regime where deteriorating shift occurs but $\epsilon_q - \epsilon_q \le 0$. As a negative result, 942 the following theorem states that in such cases the statistical power of the test is low.

Theorem A.9. When deteriorating shift occurs and $\epsilon_q \leq \epsilon_p$, for a chosen significance level of α , the 944 statistical power of the test in Alg. 2 is $\mathcal{O}(\alpha)$.

Proof. From the proof of Theorem. 4.4 we have

$$\text{TPR} \ge (1 - \beta) \left(1 - \mathcal{O} \left(\exp \left(-n\epsilon_0^2 + d \right) \right) \right)$$
(68)

$$\beta := \Pr\left[\left\{\widehat{\operatorname{err}}(h; \boldsymbol{Q}_f) \le \mu\right\} | \left\{h \in \mathcal{H}_p\right\}\right]$$
(69)

Using A.2 on \boldsymbol{P} and α we get

$$\alpha \in \mathcal{O}(\exp\left(-n(\mu - \epsilon_p)^2 + d_p\right)) \tag{70}$$

Using A.2 on Q we get

$$\Pr\left(\left\{\widehat{\operatorname{err}}(h; \boldsymbol{Q}_f) \ge \mu\right\} \mid \{h \in \mathcal{H}_p\}\right) \in \mathcal{O}\left(\exp\left(-n(\mu - \epsilon_q)^2 + d_p\right)\right)$$
(71)

$$1 - \beta \in \mathcal{O}\left(\exp\left(-n(\mu - \epsilon_q)^2 + d_p\right)\right) \tag{72}$$

$$1 - \beta \in \mathcal{O}\left(\alpha\right) \tag{73}$$

The last equation follows since we are dealing with the case where $\epsilon_p \ge \epsilon_q$. Thus, the TPR is $\mathcal{O}(\alpha)$ irrespective of the magnitude of n, as desired.

972 B EXPERIMENTAL SETUP AND ADDITIONAL DETAILS 973

974 B.1 THE BAYESIAN PERSPECTIVE 975

976Crucial to the effective functioning of D-PDDM is the signal coming from the training set. It is this977signal with which disagreement rates are computed in both D-PDDM pre-training and D-PDDM978testing, as it serves as a "grounding" for the subsequent disagreement optimization in that one forces979disagreement on a held-out validation set of choice which may or may not be in-distribution while980constraining oneself to respect the training dataset. D-PDDM effectively translates this signal from981the training set into a constrained hypothesis space \mathcal{H}_p which gets outputted upon the completion of982pre-training, thus avoiding the need to store the training dataset.

983 One can view the hypothesis space of a parametrized family as the parameter space themselves, 984 though this is not yet enough. Even when one is able to represent \mathcal{H}_p , it then becomes a question of representing the restriction to this parameter space, i.e. fence the set of parameters such that models 985 in this set perform well on the training dataset. To this, we propose a soft style of fencing by viewing 986 the training of the base model from the Bayesian perspective. Specifically, in addition to optimizing 987 the parameters of f, one also optimizes the posterior belief over the parameter space conditional on 988 having observed the training data. Thus, lines 5 in Algorithm 1 and 2 of Algorithm 2 can be roughly 989 approximated by sampling from the posterior. 990

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Maximum disagreement rate posterior sampling. Let \mathcal{H} be parametrized by \mathcal{W} with some prior belief P(w), denote the training dataset by \mathcal{D}^n . Upon training from \mathcal{D}^n , we update our belief over the weights of the model parameters via the posterior distribution $P(w|\mathcal{D}^n)$. For the pre-training step, let \mathcal{D}^m be the in-distribution sample to disagree on at some round $t \leq T$. In order to approximate a disagreement rate conditional on our posterior, we sample weights $\{\tilde{w}_i\}_{i=1:K} \sim P(w|\mathcal{D}^n)$. Then, for each tentative weight \tilde{w}_i , we compute the tentative disagreement rate $\tilde{\phi}_i = \widehat{\operatorname{err}}(h(\cdot; \tilde{w}_i); \mathcal{D}^m)$ on \mathcal{D}^m . Finally, $\max_{i=1:K} \tilde{\phi}_i$ is appended to Φ . The exact same sampling procedure is used in Algorithm 2

in order to compute one disagreement rate ϕ_Q from $\mathcal{D}^m \sim Q$ where $P \stackrel{?}{=} Q$, where the algorithm 999 identifies whether ϕ_{Ω} lies beyond the $(1 - \alpha)$ -quantile of Φ . Effectively, although we do not solve 1000 exactly for the maximum disagreement rate achievable in the restricted family, we trade off this 1001 hard constraint requiring a potentially complicated optimization mechanism with an approximate 1002 lower-bound maximum sampling scheme by taking the empirical maximum disagreement rate from 1003 K different posterior weight samples. It is also important to emphasize that this procedure implicitly 1004 relaxes the adherence on candidate auxiliary functions h with weights w having to be at least as good 1005 as f on \mathcal{D}^n . Even with a concentrated posterior, the support of $P(w|\mathcal{D}^n)$ would still cover \mathcal{W} and although unlikely, there is a possibility of sampling weights w for which $h(\cdot; w)$ does not achieve the theoretical desired accuracy ϵ . The result is, however, a very efficient sampling scheme where 1. we 1008 rely on the concentration of $P(w|\mathcal{D}^n)$ so that sampling extremely bad weights occurs rarely, and 2. 1009 we rely on a large K in order to lower-bound the true maximum disagreement rate.

1010 1011 It is also worth mentioning that sampling from $P(w|\mathcal{D}^n)$ can be done via Markov Chain Monte Carlo, Langevin dynamics, variational inference, etc... Our implementation uses variational inference as it was found to be the fastest, though results may vary.

1013 1014

Large models and very large models. Though Algorithms 1 and 2 are largely theoretical, when viewed from the Bayesian perspective, the approximate optimization becomes tangible. When \mathcal{H} is the family of neural networks on tabular features, the implementation effectively becomes Bayesian neural networks (Bishop, 1997). For neural networks accommodating various structural inductive biases on the data such as convolutional nets, recurrent nets, and potentially transformer architectures, per Harrison et al. (2024) it is possible to trade-off little to no performance in exchange for efficiency by modeling the distribution of parameters only on the last classification layer, thereby avoiding most of the variational inference on the feature extraction layers.

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Training dataset compression. One may view the information content provided by the training set
 as being condensed into the constrained hypothesis space. We argue that for deep models trained on
 datasets of tens or hundreds of millions of samples, the storage and computation of disagreement
 rates represents a bottleneck in the efficient monitoring of algorithms. In training the models to

1026 disagree, not only is the practitioner performing forward passes of the entire training set but also 1027 backpropagating the disagreement objective in order to finetune a version of the model from which a 1028 maximal disagreement rate is computed and appended to Φ . Even when one entirely pretrains on 1029 more powerful HPC clusters, one is still left to run the D-PDDM test on a local machine monitoring 1030 the deployment of f. When considering monitoring language models or multimodal models in high-1031 stakes environments for instance, both the training data storage and the backpropagation becomes a 1032 challenge.

1033 The literature on coresets (Mirzasoleiman et al., 2020; Bachem et al., 2017; Karnin & Liberty, 2019; 1034 Feldman, 2020) provides a candidate solution to this problem. By sampling a small subset consisting 1035 of the most representative samples of the training set, one effectively compresses the information of 1036 the training set into rough representatives of the different classes. Similarly, the literature on prototype learning (Snell et al., 2017; Biehl et al., 2016; Xu et al., 2020; Deng et al., 2021) provide a similar 1037 style of information compression. In particular, prototypical ensembles may be employed where each 1038 ensemble member captures specific particularities of the training set, faithfully compressing not only 1039 the "average" but also the irregularities of the data manifold. 1040

1041 It could be worthwhile to consider \mathcal{H}_p as feature representations of the training set instead. The entire 1042 training set is compressed via its feature representation which may be trained from supervision or 1043 in a semi-supervised fashion. This style of compression is conditional on having learned general 1044 representation of the dataset, the latter may be transfer learned from pretrained weights of similar 1045 tasks. In all of the aforementioned cases, one is still left to backpropagate during both pre-training as 1046 well as D-PDDM test. The Bayesian perspective avoids this entirely by offloading its computation 1047 into the approximate sampling scheme which can be done efficiently.

1049 B.2 SYNTHETIC DATA GENERATION

For all experiments, let d be the number of features. To generate a P_g -distributed dataset centered at $\mu \in \mathbb{R}^{d-1}$ with isotropic variance σ_1^2 , (d-1)-dimensional samples are generated from a Gaussian distribution with mean μ and covariance $\sigma_1^2 \cdot I_{d-1}$. For n (d-1)-dimensional samples $\{x^{(i)}\}_{i=1}^n$ with $x^{(i)} = (x_1^{(i)}, \dots, x_{d-1}^{(i)})$, we compute their d^{th} features according to

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with $\theta^{(i)} \sim \mathcal{N}(0, \sigma_2^2), \Delta \ge 0$ is a gap parameter, and x is then assigned the label $\operatorname{sgn}(\theta^{(i)})$. Effectively our samples lie above and below a sinusoidal hypersurface decision boundary and are concentrated near $(\mu, \sum \sin(\mu_i))$, with Δ controlling the minimum orthogonal distance from our samples to the decision boundary. In all experiments, we choose $\sigma_1^2 = \sigma_2^2 = 1$, and $\mu = \pi \cdot I_{d-1}$. For all experiments, the true positive rate (TPR) is reported at level $\alpha = 0.05$. In deteriorating shifts, we set $\Delta = 0$ while in non-deteriorating shifts, we set Δ to vary smoothly.

 $x_d^{(i)} = \sum_{i=1}^{d-1} \sin(x_i^{(i)}) + \theta^{(i)} + \operatorname{sgn}(\theta^{(i)}) \cdot \Delta$

B.3 INDUCING SHIFTS

1068 **Deteriorating shift.** Deteriorating shift is induced by shifting μ along the (d-1)-dimensional 1069 1-vector by a factor of ζ which we smoothly control. From the data generation process, the first 1070 (d-1) dimensional covariates are shifted and consequentially, the d-th covariate as well. We denote 1071 this shifted distribution by Q_x . Effectively, this generates data centered near a different region of the decision boundary that the base classifier would not have seen and is unlikely to have been able 1072 to generalize to given the P_q -distributed training data. In fact, as shown by Figure 5, we remark 1073 that it is highly unlikely that base classifiers could generalize the periodic property of the decision 1074 boundary given the low variance of the x_1 coordinate unless the hypothesis class exclusively contains 1075 periodic functions. Therefore, performance drop is expected for any base classifier that learns from 1076 the P_q -distributed training samples. 1077

1078 Non-deteriorating shift. Non-deteriorating shift for the test distribution Q_x is induced by evenly 1079 mixing samples from P_g generated using $\Delta = 0$ with samples generated using $\Delta > 0$. This has the effect of stretching the centroids of the positively and negatively labeled points away from the



Figure 7: Data generation visualization in 2-dimensions. Samples generated from P_x are colored red, while samples generated from Q_x are colored blue. Samples above the sine curve are positively labeled, while those underneath are negatively labeled. The means of the first coordinates of distributions P_x and Q_x are labeled and colored accordingly. In practice, we analogously slide the mean of Q_x progressively to the right by ζ to induce deteriorating shift. The induction of non-deteriorating shift has an effect of stretching the distributions along the y-axis in the image as a function of the gap parameter Δ .

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decision boundary along the d^{th} coordinate axis. A base classifier trained on P_g should perform similarly on Q_x . We should expect a good PDD monitoring algorithm to enjoy low false positive rates under under this setup.

B.4 ADDITIONAL SYNTHETIC RESULTS ON DETERIORATING SHIFT



Figure 8: Analysis. (a) Across multiple base classifiers of differing qualities, the algorithm enjoys
 acceptably low FPRs when exposed to non-deteriorating shifts. (b) Base classifiers of differing
 qualities are able to effectively detect deteriorating shift and achieve high TPRs.

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Deteriorating shift: effectiveness of the D-PDDM. We vary the amount of data shift in the x-axis for differing qualities (ϵ_f) of the base classifier in Fig. 8 (b). For each base classifier, as the shift increases the test is better able to detect the deterioration. Note that deterioration in the shifts can be written as $\xi = \text{TV} - 2\eta$ (from 5). The x-axis quantifies the amount of shift. However, the deterioration also depends on η (see 6) which is different for each base classifier (even for fixed shift) due to differing ϵ_f . Hence, for a specific data shift, the deterioration can differ across base classifiers. We see the effect of this in 8 (b). In general, from 4.4, the trend is that a better base classifier (lower ϵ_f) has higher TPR. For a particular shift, due to the difference in η deterioration (ξ) could be different resulting in some deviation from the general trend. This highlights how 4.4 captures several of the subtle complexities of D-PDD.

1139 B.5 BASELINES DETAILS

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1141 We compare our disagreement-based hypothesis test algorithm against several other methods from the 1142 literature that either detect distribution changes or can be converted into a PDD monitoring protocol. 1143 Let $X = \{x^{(i)}\}_{i=1}^{n}$ from P_x and $Y = \{y^{(i)}\}_{i=1}^{m}$ from Q_x be given. These algorithms seek to accept 1144 or reject the hypothesis that $P_x = Q_x$ in distribution.

- 1. Deep Kernel MMD (Liu et al. (2020)) The algorithm first learns a deep kernel by optimizing a criterion which yields the most powerful hypothesis test. With this learned kernel, permutation tests are run multiple times in order to determine a true positive rate for the algorithm. We interface the authors' original source code with our repository and recycle their training procedures. Theirs can be found at https://github.com/fengliu90/DK-for-TST.
- 1151 2. H-Divergence (Zhao et al. (2022)) The algorithm fits Gaussian kernel density estimates for 1152 P_x, Q_x , and their uniform mixture $(P_x + Q_x)/2$. Then, permutation tests are performed 1153 using the test statistic $H_{\ell}((\mathbf{P}_x + \mathbf{Q}_x)/2) - \min\{H_{\ell}(\mathbf{Q}_x), H_{\ell}(\mathbf{P}_x)\}$ where H_{ℓ} is the H-1154 entropy with $\ell(x, a)$ the negative log likelihood of x under distribution a estimated by the 1155 Gaussian kernel density, in order to determine a true positive rate for the algorithm. This 1156 test statistic is an empirical estimate of the H-Min divergence. The choice of the particular H-divergence is a hyperparameter and is problem dependent, as well as the choice for how 1157 to generatively model the data distributions. The original paper further experimented with 1158 fitting Gaussian distributions as well as variational autoencoders (VAEs), both of which are 1159 not explored here. We interface the authors' original source code with our repository. Theirs 1160 can be found at https://github.com/a7b23/H-Divergence/tree/main. 1161
- 11623. f-Divergence (Acuna et al. (2021)) f-divergence generalizes several notions of distances1163between probability distributions commonly used in machine learning. In this paper, we
convert the Kullback-Leibler (KL) and the Jensen-Shannon (JS) divergences, particular
cases of f-divergences, into permutation tests. More specifically, we first fit Gaussians on
samples coming from P_x and Q_x using maximum likelihood. In the case of KL-divergence,
the empirical KL-divergence is computed between the fitted Gaussians whereas for the
JS-divergence, we fit an additional Gaussian on the mixture distribution M and leverage the
identity:

$$JS(\boldsymbol{P}_{x}||\boldsymbol{Q}_{x}) = \frac{1}{2}(KL(\boldsymbol{P}_{x}||\boldsymbol{M}) + KL(\boldsymbol{Q}_{x}||\boldsymbol{M}))$$

We run permutation tests by permuting the samples in the union $(X \sim P_x^n) \cup (Y \sim Q_x^m)$. It is worth noting that as with H-divergence, more elaborate generative models could be fitted onto samples X and Y, which we do not explore in this work.

- 4. Black Box Shift Detection (BBSD) (Lipton et al., 2018) involves estimating the changes in the distribution of target labels p(y) between training and test data while assuming that the conditional distribution of features given labels p(x|y) remains constant. This is achieved by using a black box model's confusion matrix to identify discrepancies in the marginal label probabilities between the training and test distributions, allowing detection and correction of the shift.
- 11805. Relative Mahalanobis Distance (RMD) (Ren et al., 2021) RMD modifies the traditional
Mahalanobis Distance (MD) for out-of-distribution (OOD) detection by accounting for
the influence of non-discriminative features. It subtracts the MD of a test sample to a
background class-independent Gaussian from the MD to each class-specific Gaussian,
effectively isolating discriminative features and improving OOD detection, especially for
near-OOD tasks. We test for shift by performing a KS test directly on the distribution of the
RMD confidence scored computed on Q_x and P_x .
- 1187 Importantly, most baselines perform some comparison using distances in covariate space. Though this may be effective, they are inevitably susceptible to false positives when the

1188 shift is non-deteriorating. To the best of our knowledge, our method is the first deteriorating 1189 shift detection method which resists flagging non-deteriorating shifts due to leveraging the 1190 disagreement statistics which help the model mitigate FPRs down the line, as the auxiliary 1191 models would not disagree any better than the base model out-of-distribution when the distribution does not result in model deterioration. 1192

1194 B.6 THE GEMINI DATASET

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GEMINI Study and Preprocessing. The General Medicine Inpatient Initiative (GEMINI) study is a 1196 retrospective cohort study of adult patients and their clinical and administrative data (Verma et al., 1197 2021). This analysis used data from over 200,000 patients from the GEMINI Database, spanning 7 1198 different hospitals that participated in the GEMINI Study. Each patients information is processed 1199 into 900 features including but not limited to: (i) laboratory results and vital results collected up to 1200 48-hours after admission, split into 6 hour intervals, (ii) patient demographic information: age, sex 1201 etc, (iii) Patient diagnosis using ICD-10-CA codes. Missing feature values are imputed based on 1202 simple averaging. The predictive task related to this data is to predict 14-day mortality for patients 1203 based on these collected features.

1204 **Data Splitting and Shift.** Based on this pre-processed data, 2 shifts are analysed: (i) temporal shift, 1205 and (ii) age-group shift. The temporal shift analysis splits data into half-years - 2018H1, 2019H2, etc. 1206 The baseline model uses 2017H1 and prior data for training, and 2017H2 for validation; Tab. 3 shows 1207 patient statistics for this split. It is subsequently tested on unseen in distribution data and later splits. 1208 The different age groups are created by splitting the data into 5 equally sized groups based on ages of 1209 patients: (1) 18-52, (2) 52-66, (3) 66-72, (4) 76 - 85, (5) 85+; Tab. 4 shows patient statistics for this 1210 split. The reported analysis trains a baseline model on group 1 (18-52) and then tests on test-sets that 1211 contain some portion of data from the 5th group (85+) and the remaining as unseen in distribution data. The portions [0.0, 0.2, 0.4, 0.6, 0.8, 1.0] represent what percentage of the test set is ood (from 1212 group 5), whilst the remaining amount is iid (from group 1). For example a ratio of 0.2 means 20% 1213 of the test data is from group 5(ood) whilst 80% is from group 1(iid). We chose to experiment on 1214 such portions instead of just subsequent age groups as this process better displays the True Positive 1215 Detection Rate of our method as well as baselines w.r.t degree of shift / perfromance deterioration. 1216

1217 Model and Method Hyper-Parameters. The base models used were neural networks with hidden 1218 layers [128, 64, 32, 16] and were trained to predict 14 day mortality on patients given the aforementioned co-variates. The hyper parameters of the model and method were fixed to be the same 1219 for both the age and temporal contexts to ensure fairness of results, thus showing that at a fixed 1220 sensitivity, the method is able to differentiate between deteriorating and non-deteriorating shifts. 1221 Our recommendation is to use a control test-set with a known deterioration in order to tune hyper 1222 parameters to desired sensitivity to distribution shift. 1223

Year	Patient Coun	t Label Ratio
Pre-201	7 72316	3.99%
2017H2	17208	3.60 %
2018H1	18233	4.15%
2018H2	18469	3.83%
2019H1	19041	3.50%
2019H2	18601	3.49%
2020H1	15575	4.50%
2020H2	11155	3.48%
2021H1	10625	3.46%
2021H2	7396	2.95%

Age	Patient Count	Label Ratio
18-52	33220	0.82 %
52-66	33146	2.36 %
66-72	31048	3.36 %
76 - 85	34055	4.77 %
85+	32399	7.82 %

 Table 4: Age Split Data Summary

Table 3: Temporal Split Data Summary

1239 STATEMENT ON THE USAGE OF COMPUTING RESOURCES **B**.7

All experiments were run on High Performance Computing (HPC) clusters. For our algorithm as 1241 well as some of the baselines, neural networks used as function approximators are implemented in PyTorch and trained on GPU-enabled nodes. The requested memory for all compute jobs was 16G each, but we believe the jobs are able to run with much less memory. Time of execution was not documented throughout the process.