

000 001 002 003 004 005 006 007 008 009 010 011 012 013 014 015 016 017 018 019 020 021 022 023 024 025 026 027 028 029 030 031 032 033 034 035 036 037 038 039 040 041 042 043 044 045 046 047 048 049 050 051 052 053 TOWARDS SCALABLE AND ROBUST FILTRATION LEARNING FOR POINT CLOUDS VIA PRINCIPAL PER- SISTENCE MEASURE

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ABSTRACT

Topological features in persistent homology extracted via a filtration process have been shown to enhance the performance of machine learning tasks on point clouds. The performance is highly related to the choice of filtration, thereby underscoring the critical significance of filtration learning. However, current supervised filtration learning method for point clouds can not scale well. We identify that this shortcoming stems from the utilization of Persistence Diagrams (PD) for encoding topological features, such as connected components, rings or voids, etc. To address this issue, we propose to use Principal Persistence Measure (PPM), an existing statistical approximation of PD, as an alternative representation and adapt existing network for PPM-based filtration learning. Experimental results on point cloud classification task demonstrate the effectiveness, scalability and robustness of our PPM-based framework.

1 INTRODUCTION

Topological information is shown to be effective in machine learning tasks on point clouds across many fields, such as biology (Kovacev-Nikolic et al., 2016; Liu et al., 2022; Meng et al., 2020; Xia et al., 2018; Xia & Wei, 2015) and chemistry (Hiraoka et al., 2016; Lee et al., 2017; Townsend et al., 2020). Topological features of a point cloud are built from a nested sequence of simplicial complexes (Sahnikov et al., 2018) called *filtration*. The birth ($b_i \in \mathbb{R}$) and death ($d_i \in \mathbb{R}$) of a cycle, e.g., a ring (1-dimensional cycle) or a void (2-dimensional cycle), of the sequence are encoded in *Persistence Diagram* (PD) $\mathcal{D} = \{r_i = (b_i, d_i) \in \Omega | 1 \leq i \leq N(\mathcal{D})\}$, where **each $r \in \mathcal{D}$ is defined as a topological feature corresponding to the cycle**, $\Omega = \{(t_1, t_2) \in \mathbb{R}^2 | t_2 > t_1\}$ is an open half-plane and $N(\mathcal{D})$ is the number of topological features. PD can be transformed into a vector and fed into a machine learning model as input. A brief illustration of PD-based pipeline for point cloud¹ is shown in Figure 1(a,b,d,f).

In the pipeline, despite different learnable vectorization methods like Carrière et al. (2020); Kim et al. (2020); Reinauer et al. (2021), it is shown in Nishikawa et al. (2023) that the final performance is highly affected by the choice of the filtration. In addition, although there are different unsupervised filtration choices like Rips (Hausmann et al., 1995), DTM (Fasy et al., 2018) and Λ -filter (Zhang et al., 2023), supervised filtration learning (Nishikawa et al., 2023) for point cloud often produces better results. We will refer this PD-based pipeline with filtration learning as PD-FL for short.

Based on weighted filtration, PD-FL (Nishikawa et al., 2023) develops a neural network architecture with isometry-invariance to learn the weight in an end-to-end way. However, since the computation algorithm² of filtration-induced PD is highly nontrivial to parallelize and can only be conducted by either pure CPU implementations (Bauer, 2021; Pérez et al., 2021) or a CPU-GPU hybrid one

¹Note that this pipeline can also be used for graph data, where the filtration usually employs unsupervised characteristics of a graph like degree (vertex-level), Ricci curvature (edge-level)(Ballester & Rieck, 2023; O’Bray et al., 2021; Southern et al., 2023) or outputs of supervised learnable networks (Hofer et al., 2020; Horn et al., 2022; Immonen et al., 2023; Mukherjee et al., 2024; Zhang et al., 2022). In this paper, we focus on the pipeline for point cloud.

²As pointed by Zomorodian & Carlsson (2004), time complexity for computing PD in the worst case is $O(m^3)$, where m is the number of simplices in the filtration. If we want topological feature corresponding to

(AIDOS-Lab; Zhang et al., 2020), this network suffers from high time cost and can not scale for a large point cloud.

In order to address this issue, we propose to replace PD in the pipeline with Principal Persistence Measure (PPM) (Gómez & Mémoli, 2024; Tung et al., 2025), which is a statistical approximation of PD, for the following two reasons: 1) As shown in Tung et al. (2025), PPM can be computed entirely on GPU in a parallel way, making it ideal for a scalable filtration learning framework. 2) PPM can capture topological information in a point cloud. PPM has been used in Tung et al. (2025) for latent space matching in Generative Adversarial Networks (Goodfellow et al., 2020). Although PPM is a rather vague approximation of PD and may not demonstrate all the possible topological features in a point cloud because the sampling mechanism favors points in dense region, the experiments in Figure 2 of Tung et al. (2025) demonstrate that a smaller distance (measured by Persistence Weighted Gaussian Kernel (Kusano et al., 2016) based Maximum Mean Discrepancy) between two PPMs indicates a smaller Wasserstein distance between the PDs. This shows that topological information can be obtained through PPM.

The main contributions of this work are threefold:

1. Propose to use Principal Persistence Measure (PPM) in filtration learning framework (Nishikawa et al., 2023) to addresses the scalability limitation of PD-based approach and adapt existing framework for PPM-based Filtration Learning (PPM-FL).
2. Establish the theoretical guarantee on the robustness of PPM against outliers and perform corresponding experimental validation.
3. Demonstrate the effectiveness and scalability of our proposed PPM-FL in point cloud classification task on public datasets.

The notations are summarized in Table 1.

Table 1: Notations.

Notation	Type	Description
X	Point Cloud	Finite point cloud sampled from a k -dimensional manifold $\mathcal{M} \subset \mathbb{R}^d$
X_η^g	Sublevel Set	Sublevel set of X at scale η for filter function $g : X \rightarrow \mathbb{R}^+$
$\mathcal{K}(X)$	Filtration	Nested sequence of topological spaces $\{X_\eta^g\}_{0 \leq \eta < \infty}$
\mathcal{D}	Persistence Diagram (PD)	Multiset of topological features $\mathcal{D} = \{r_i = (b_i, d_i) \in \Omega \mid 1 \leq i \leq N(\mathcal{D})\}$, where b_i is birth, d_i is death of a cycle
Ω	Open Half Plane	$\Omega = \{(t_1, t_2) \in \mathbb{R}^2 \mid t_2 > t_1\}$
r_i	Topological Feature	$r_i \in \mathcal{D} \subset \Omega$
$N(\mathcal{D})$	Count	Number of topological features in PD
q	Homology Dimension	Dimension of cycles
$w(\cdot)$	Weight Function	Weight function for weighted filtration
\mathbb{X}_s	Subset Collection	$\mathbb{X}_s = \bigcup_{i \in [M]} X_s^i$, where $X_s^i \subset X$ is a random subset of size $2q + 2$
M	Count	Number of random subsets in PPM
$\bar{\mu}$	Empirical EPD	Average measure of PDs from random subsets: $\bar{\mu} = \frac{1}{M} \sum_{i=1}^M \mu_i$
μ_i	Sampled PD	Dirac measure for PD of subset X_s^i (sampled PD): $\mu_i = \sum_{j=1}^{N(\mathcal{D}_i)} \delta_{r_j}$, δ_{r_j} is the Dirac point mass at topological feature r_j
P_o	Contaminated Distribution	$P_o = (1 - \epsilon) \cdot P + \epsilon \cdot U$, P is inlier density, U is outlier density and ϵ is the outlier percentage

2 BACKGROUND

We provide the relevant information about Persistence Diagram and weighted filtration (refer to Chazal & Michel (2021) for a comprehensive introduction).

1-dimensional cycle (ring), we need to consider up to 2-simplices in the complex. The number of simplices is $O(n^3)$ and the computational cost can be up to $O(n^9)$, where n is the size of the point cloud.

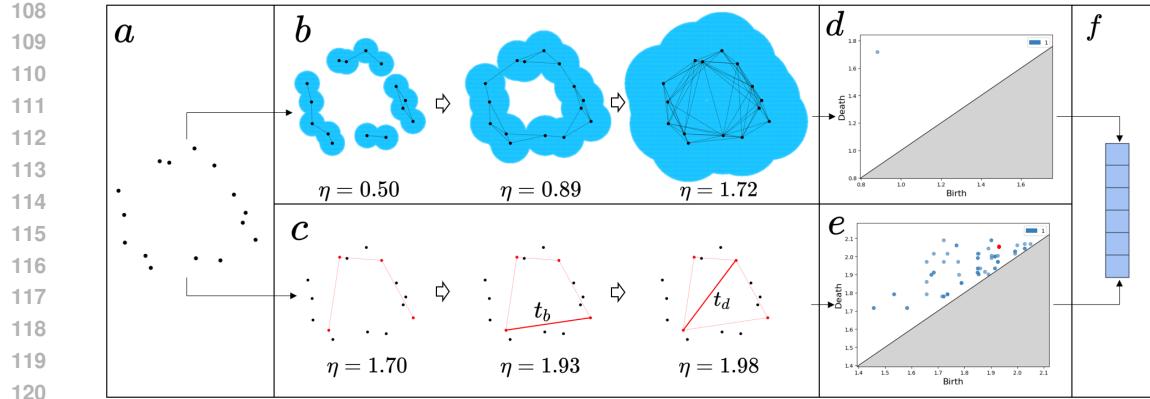


Figure 1: PD (a,b,d,f) and PPM-based (a,c,e,f) pipeline for point cloud. (a) Original point cloud X . Note that this can also be a distance matrix, since in the construction of simplicial complexes of the filtration, a pairwise connection is added if the pairwise distance is lower than a threshold η . This can be equivalently expressed that for balls centered at each point with radius of $\eta/2$, if two balls touch, an edge between two balls’ centers is added. (b) An example filtration (Rips filtration) at values of η of X . The union of balls is intended to show the process of the Rips filtration: when two balls touch (pairwise distance $\leq \eta$), an edge is added. According to Nerve theorem (Mona & Hintz, 2023), $X_\eta = \bigcup_{x \in X} B(x, \eta/2)$ is actually homotopy equivalent to Čech complex. While the Rips filtration serves as a practical approximation of the Čech filtration, it does not strictly reflect the topology of the union of balls. (c) An example filtration (Rips filtration) at various values of η of one subset of X . The distances of the bold lines are t_b and t_d . (d) 1-dimensional Persistence Diagram of X . (e) 1-dimensional Principal Persistence Measure of X . **The red point corresponds to the topological feature obtained via the red subset in (c).** (f) Vectorization of PD or PPM.

2.1 PERSISTENCE DIAGRAM

Let $g : \mathcal{X} \rightarrow \mathbb{R}^+$ denote a function on space \mathcal{X} , where \mathbb{R}^+ stands for positive real numbers, \mathcal{X} is a bounded and open subset of Euclidean space. Function g is computed based on a finite point cloud X sampled from manifold $\mathcal{M} \subset \mathcal{X}$. **This manifold assumption means that the finite point cloud X is sampled from an underlying k -dimensional manifold \mathcal{M} , where $\mathcal{M} \subset \mathbb{R}^d$ is a smooth, low-dimensional subspace embedded in a higher-dimensional Euclidean space \mathbb{R}^d .** At scale $\eta \geq 0$, the sublevel set $\mathcal{X}_\eta^g = \{x \in \mathcal{X} \mid g(x) \leq \eta\}$ encodes the topological information in \mathcal{X} . For $\gamma \leq \eta$, we can have the nested sublevel sets $\mathcal{X}_\gamma^g \subseteq \mathcal{X}_\eta^g$. By increasing scale η from 0, we obtain a filtration $\mathcal{K}(X) = \{\mathcal{X}_\eta^g\}_{0 \leq \eta < \infty}$, a nested sequence of topological spaces.

A cycle is considered ‘born’ at $b \in \mathbb{R}$ when it first emerges in \mathcal{X}_b^g , and it ‘dies’ at $d \in \mathbb{R}$ when it ceases to exist in \mathcal{X}_p^g for any $p > d$. 0-dimensional cycles are connected components; 1-dimensional cycles are rings or loops; 2-dimensional cycles are voids, etc. This homology dimension is denoted as q . Topological feature $r = (b, d)$, which corresponds to a cycle, is presented in the form of PD $\mathcal{D} = \{r_i = (b_i, d_i) \in \Omega \mid 1 \leq i \leq N(\mathcal{D})\}$, where $N(\mathcal{D})$ is the number of topological features. An example using Rips filtration (Hausmann et al., 1995) $g(\cdot) = 2 \min_{x \in X} \ell(\cdot, x)$, where ℓ is Euclidean distance, and corresponding PD are provided in Figures 1(b) and 1(d). **In practice, we usually set the maximum threshold for the filtration to be a finite value or just remove the point with infinite death time since it exists for all point clouds and has no practical value.**

2.2 WEIGHTED FILTRATION

In Rips filtration, at scale η , the sublevel set is $\mathcal{X}_\eta = \bigcup_{x \in X} B(x, \eta/2)$, where $B(x, \eta/2)$ is the ball centered at x with radius $\eta/2$. Each ball has the same radius. Weighted filtration aims to put weight on each point’s corresponding radius. For weighted filtration, at scale η , the sublevel set is $X_\eta = \bigcup_{x \in X} B(x, \eta - w(x))$, where $w(\cdot) : X \rightarrow \mathbb{R}$ is the weight function. Current work (Nishikawa et al., 2023), i.e., PD-FL, designed a network to learn this weight function w . **In order to align with the setting in PD-FL and ensure a fair comparison, our work is also based on the weighted filtration.**

162

3 RELATED WORK

164

3.1 FILTRATION LEARNING

166 Supervised filtration learning is first introduced for graph data³ by designing learnable vertex filter
 167 function (Hofer et al., 2020). It is then studied for more extensive and general purposes on graph
 168 data (Horn et al., 2022; Immonen et al., 2023; Mukherjee et al., 2024; Zhang et al., 2022). Filtration
 169 learning for point cloud is rarely developed. Existing work (Nishikawa et al., 2023) built a network
 170 via weighted filtration, i.e., given a point cloud $X \subset \mathbb{R}^d$, one can define the radius value $r_x(\eta)$ at
 171 scale η for $x \in X$ as $r_x(\eta) = \eta - w(x)$ if $\eta > w(x)$, otherwise $r_x(\eta) = -\infty$, where w is the
 172 weight function. DTM (Fasy et al., 2018) is a special case of this weighted filtration where w is
 173 distance-to-measure function.

174 It is required in Nishikawa et al. (2023) that for filtration learning, the weight function $w(\cdot) =$
 175 $f(X, \cdot) : \mathbb{R}^d \rightarrow \mathbb{R}$ needs to meet the following three conditions:

- 176 1. f should be determined by the whole point cloud X and does not depend on the order of the
 177 points in X ;
- 178 2. f should be isometry-invariant, i.e., for any isometric transformation T , any point cloud X ,
 179 and $x \in X$, $f(TX, Tx) = f(X, x)$;
- 180 3. The output of the $f(X, x)$ should have both of global information X and pointwise informa-
 181 tion of x .

183 A network⁴ that relies on deepsets (Zaheer et al., 2017) and takes distance matrix as input is de-
 184 signed to satisfy the conditions above. Once the filtration is determined by this network, PD of the
 185 entire point cloud is computed and then can be vectorized as input to a Multi-Layer Perceptron for
 186 classification task. Although this network outperforms unsupervised filtration like Rips and DTM,
 187 it relies on CPU for the computation of PD and the substantial time cost (Zomorodian & Carlsson,
 188 2004) for computing PD prevents its scalability.

190

3.2 PRINCIPAL PERSISTENCE MEASURE

192 One way to reduce the time cost of computing PD of the entire point cloud is to use statistical
 193 approximation: for multiple random subsets⁵ (with fixed size) of the entire point cloud X , a PD
 194 $\mathcal{D}_i = \{r_j = (b_j, d_j) \in \Omega | 1 \leq j \leq N(\mathcal{D}_i)\}$ is obtained for each random subset $X_s^i \subset X$. The
 195 statistical approximation, i.e., Expected PD (EPD) (Chazal & Divol, 2018), takes a distributional
 196 view and represents each PD of subset X_s^i as a measure $\mu_i = \sum_{j=1}^{N(\mathcal{D}_i)} \delta_{r_j}$ supported on Ω where δ_{r_j}
 197 is Dirac point mass at r_j . The empirical EPD is then the average $\bar{\mu} = \frac{1}{M} \sum_{i=1}^M \mu_i$, where M is the
 198 number of random subsets.

199 Principal Persistence Measure (PPM) (Gómez & Mémoli, 2024) is a special case of Expected PD
 200 where each subset X_s^i has fixed size $2q+2$ where q is the homology dimension ($q = 0$ for connected
 201 component, $q = 1$ for rings, etc.). It is guaranteed that each PD on $2q+2$ points has at most one
 202 single topological feature $r_1 = (t_b, t_d)$ when $q \geq 1$, i.e., $|N(\mathcal{D}_i)| \leq 1$, which can be efficiently
 203 computed as follows: given any $x \in X_s^i$, let $x^{(1)}, x^{(2)} \in X_s^i$ be the points such that $d(x, x^{(1)}) \geq$
 204 $d(x, x^{(2)}) \geq d(x, a)$ for any $a \in X_s^i \setminus \{x^{(1)}, x^{(2)}\}$ where d is a distance function (filtration), then

$$r_1 = (\max_{x \in X_s^i} d(x, x^{(2)}), \min_{x \in X_s^i} d(x, x^{(1)})).$$

208 PPMs have stability with respect to Wasserstein distance, as shown in Theorem A.2. The computa-
 209 tion of PPM can be easily implemented in a parallel way and conducted on GPU and the existence
 210 of r_1 is discussed in Theorem A.3. By considering random subsets, the computation of PPM costs
 211 less time than computing PD on the entire point cloud.

213 ³Filtration Learning on graph data is scalable due to the simplicity of computing PD on graph. In the
 214 filtration, the addition of an edge either connects two connected components or creates a ring.

215 ⁴The full architecture of network (Nishikawa et al., 2023) is shown in Appendix A.5.

216 ⁵Each point in the subset is i.i.d. sampled from the entire point cloud.

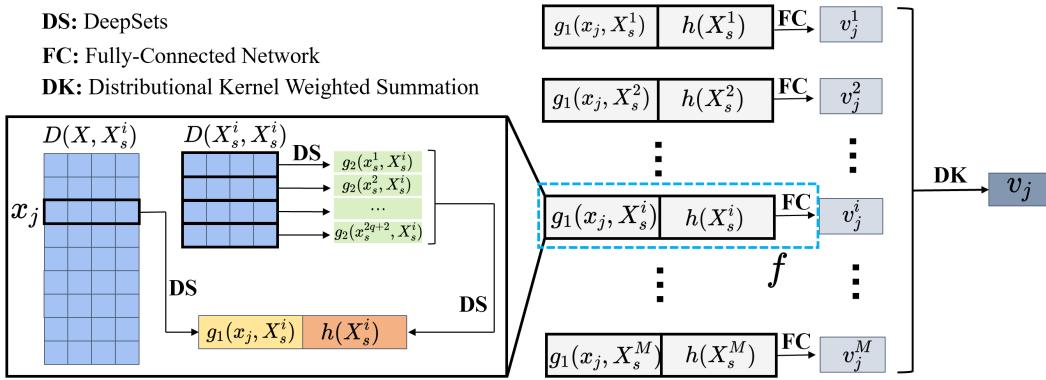
216 In order to improve scalability, we propose to use PPM, instead of PD, to encode topological information
 217 and adapt existing network (Nishikawa et al., 2023) for PPM-based filtration learning, which
 218 learns from multiple subsets.
 219

220 4 FILTRATION LEARNING FOR PPM

221
 222 We propose the filtration learning framework for PPM (PPM-FL) based on a weighted filtration.
 223 PPM-FL, which concentrates on learning from multiple subsets, is adapted from the network in
 224 Nishikawa et al. (2023) for learning from the entire point cloud.
 225

226 Different from the three conditions mentioned in Nishikawa et al. (2023), here weight function w
 227 should be related to $\mathbb{X}_s = \cup_{i \in [M]} \{X_s^i\}$, with each subset $X_s^i \subset X$ of size $2q + 2$, where q is the
 228 homology dimension, instead of the whole point cloud X . This gives the following three adapted
 229 requirements for the weight function $w(\cdot) = \bar{f}(\mathbb{X}_s, \cdot)$:

- 230 1. The output of $\bar{f}(\mathbb{X}_s, x)$ should be determined by each subset X_s^i and does not depend on the
 231 order of the points. The closer a subset X_s^i is to x , the greater its impact on x should be.
 232
- 233 2. \bar{f} should be isometry-invariant, i.e., for any isometric transformation T , any point cloud X ,
 \mathbb{X}_s and $x \in X$, $\bar{f}(T\mathbb{X}_s, Tx) = \bar{f}(\mathbb{X}_s, x)$, where $T\mathbb{X}_s \triangleq \cup_{i \in [M]} \{TX_s^i\}$
 234
- 235 3. The output of $\bar{f}(\mathbb{X}_s, x)$ should have both of global information \mathbb{X}_s and pointwise information
 236 of x .
 237



250 Figure 2: PPM-based Filtration Learning Framework. Value v_j is the output of $\bar{f}(\mathbb{X}_s, x_j)$. D
 251 represents a distance matrix for two point clouds X and Y , $D(X, Y) = (d(x_i, y_j))_{i=1, j=1}^{|X|, |Y|} \in$
 252 $\mathbb{R}^{|X| \times |Y|}$, where d is Euclidean distance.
 253

254 In order to deal with set $\mathbb{X}_s = \cup_{i \in [M]} \{X_s^i\}$, we model the weight function \bar{f} in a simple summation
 255 form, i.e., $\bar{f}(\mathbb{X}_s, \cdot) = \sum_{i=1}^M K(X_s^i, \cdot) f(X_s^i, \cdot)$, where f is used to output the weight (v_j^i) of the j -th
 256 point x_j in X w.r.t. subset X_s^i , i.e., $v_j^i = f(X_s^i, x_j)$. Function K measures the similarity between
 257 the input and subset X_s^i to meet requirement 1: the closer X_s^i is to x , the greater its impact on x .
 258 The filtration learning framework for PPM, as shown in Figure 2, is then adapted from Nishikawa
 259 et al. (2023) to meet the three new requirements:
 260

- 261 1. Following Nishikawa et al. (2023), the independence on the order of points is guaranteed by
 262 following DeepSets (Zaheer et al., 2017) architecture g_1 , g_2 and h :

$$263 g_1(x_j, X_s^i) = \phi^{(2)}(\mathbf{op}(\{\phi^{(1)}(d(x, x_j)) | x \in X_s^i\}));$$

$$264 g_2(x_s^k, X_s^i) = \phi^{(4)}(\mathbf{op}(\{\phi^{(3)}(d(x, x_s^k)) | x \in X_s^i\}));$$

$$265 h(X_s^i) = \phi^{(5)}(\mathbf{op}(\{g_2(x, X_s^i) | x \in X_s^i\})),$$

270 where x_s^k is the k -th ⁶ point in a subset X_s^i , d is Euclidean distance, $\phi^{(i)}$ s are all fully-
271 connected neural networks and op is the permutation invariant operator.

272 For each $x_j \in X$, after the weight v_j^i w.r.t. the i -th subset X_s^i is obtained, the final weight value
273 v_j is the distributional kernel weighted summation of each v_j^i , i.e., $v_j = \sum_{i=1}^M K(x_j, X_s^i) v_j^i$,
274 where $K(x_j, X_s^i) = \frac{1}{|X_s^i|} \sum_{x \in X_s^i} \kappa(x, x_j)$ and $\kappa(x, x_j) = \exp\left(\frac{-\|x-x_j\|_2^2}{2\sigma^2}\right)$.

275 2. The isometry-invariance is guaranteed by using the distance matrix as input.

276 3. The global and pairwise information are stored in h and g_1 respectively.

277 Once all the weights are obtained, the weighted filtration is used to compute the PPM of the point
278 cloud ⁷. The space cost of PPM-FL is $O((2q+2)nM + (2q+2)^2M)$, where q is the homology
279 dimension, M is the number of subset in PPM and n is the point cloud size.

280 As for the approximation ability, for weight function $\bar{f}(\mathbb{X}_s, \cdot) = \sum_{i=1}^M K(X_s^i, \cdot) f(X_s^i, \cdot)$, function f
281 is able to approximate any continuous function, as shown in Theorem 4.1 of Nishikawa et al. (2023).

282 PPM can be then vectorized ⁸ by a supervised method PersLay (Carrière et al., 2020) for a potential
283 task. For example, if the task is point cloud classification, we can input the resulting vector into
284 MLP that employs a cross entropy loss function. Due to the parallel implementation of PPM, this
285 PPM-based pipeline can be deployed on GPU to scale on a large point cloud.

289 5 ROBUSTNESS OF PPM AGAINST OUTLIERS

290 Here we demonstrate the robustness of PPM against outliers. We start by considering the robustness
291 of a general case of PPM, i.e., Expected Persistence Diagram (EPD), where the size of random subset
292 X_s is denoted as n , and then extend the result to PPM. Let \mathcal{M} denote the underlying manifold
293 of point cloud X ; P denote the density of the distribution on k -dimensional \mathcal{M} ; and U denote
294 the density of the distribution of outliers, such as a uniform distribution. Following the setting in
295 Vishwanath et al. (2020); Cai et al. (2025), the outlier-contaminated distribution P_o is expressed as

$$296 P_o = (1 - \epsilon) \cdot P + \epsilon \cdot U,$$

297 where ϵ is the percentage of outliers. X is a sample of P_o . Then we have the following lemma on
298 the robustness of EPD under the assumption that filtration \mathcal{K} meets K1-K5 requirements in Section
299 3 of Chazal & Divol (2018).

300 We have the following assumptions on P and U :

- 301 1. We assume that P and U share the same support. Regarding the manifold's support, U is a
302 (maybe uniform) distribution over the entire support of \mathcal{M} , including regions where the inlier
303 density P are very low and points have little chance to be sampled from this low density area.
304 An example is shown in Figure 16 in Gómez & Mémoli (2024). The support of P is the
305 circular area and the low density region lies at the inner part of the ring.
- 306 2. P and U are both lower and upper bounded in the support, i.e. there exist constants $\bar{c} \geq c > 0$
307 such that $\bar{c} \geq P(x) \geq c$ and $\bar{c} \geq U(x) \geq c$ for any x in the support. This assumption is
308 identical to assumption 2(ii) in Cai et al. (2025), which shares the same contamination model
309 $P_o = (1 - \epsilon) \cdot P + \epsilon \cdot U$.

310 **Lemma 5.1.** For EPD $\mathbb{E}_{X_s \sim P^n}[\nu(X_s)]$ with density μ_1 and $\mathbb{E}_{X_s \sim P_o^n}[\nu(X_s)]$ with density μ_2 , where
311 $\nu(X_s)$ is the measure form of PD $\mathcal{D}(\mathcal{K}(X_s))$, i.e., $\nu(X_s) = \sum_{r \in \mathcal{D}(\mathcal{K}(X_s))} \delta_r$, it holds that

$$312 \|\mu_1 - \mu_2\|_1 \leq C_n H_k(\mathcal{M})^n p_{n-1}(\epsilon) \epsilon,$$

313 ⁶This index k is used to differentiate two different point in subset X_s^i . We just assume a random order here
314 since the framework is permutation invariant.

315 ⁷Note that we could use the framework in Nishikawa et al. (2023), which uses the distance matrix of the
316 entire point cloud to learn the weights. But the space cost would be $O(n^2)$, which is one order of magnitude
317 higher than PPM-FL's $O((2q+2)nM + (2q+2)^2M)$.

318 ⁸Despite many methods for vectorization for PD or PPM, including supervised (Carrière et al., 2020; Kim
319 et al., 2020; Reinauer et al., 2021) and unsupervised ones (Adams et al., 2017; Bubenik et al., 2015; Chung &
320 Lawson, 2022), we choose to use PersLay (Carrière et al., 2020), a supervised vectorization that uses similar
321 structure like Deepsets for simplicity.

324 where C_n is the expected number of points in the PD built with the filtration \mathcal{K} on n i.i.d. points
 325 on \mathcal{M} , $H_k(\mathcal{M})$ is k -dimensional Hausdorff measure⁹ of \mathcal{M} and $p_{n-1}(\epsilon)$ is a polynomial of order
 326 $n - 1$ with bounded coefficients.

328 The proof is provided in Appendix B.

329 **Theorem 5.2.** For PPM $\mathbb{E}_{X_s \sim P^{2q+2}}[\nu(X_s)]$ with density μ_1 and $\mathbb{E}_{X_s \sim P_o^{2q+2}}[\nu(X_s)]$ with density
 330 μ_2 , it holds that

$$331 \|\mu_1 - \mu_2\|_1 \leq H_k(\mathcal{M})^{2q+2} p_{2q+1}(\epsilon) \epsilon,$$

332 where $H_k(\mathcal{M})$ is k -dimensional Hausdorff measure of \mathcal{M} and $p_{2q+1}(\epsilon)$ is a polynomial of order
 333 $2q + 1$ with bounded coefficients.

335 *Proof.* Following Lemma 5.1, PPM is a special case of EPD where the size of each subset is $n =$
 336 $2q + 2$, q is homology dimension. Combined with the fact that each subset of size $2q + 2$ has at most
 337 1 topological feature, i.e., $C_n \leq 1$, we can have the result above. \square

339 Theorem 5.2 indicates that a small number of outliers in the point cloud will not severely disturb
 340 PPM. [The relation between the upper bound and outlier distribution \$U\$ is discussed in Appendix](#)
 341 [B.3](#). The experimental demonstration of PPM’s robustness with the learned filtration in point cloud
 342 classification task is provided in Section 6.2. We discuss the relation between Theorem 5.2 and
 343 existing results in Divol & Lacombe (2021b) in Appendix D.4.

345 6 EXPERIMENTS

347 We compare PPM-FL with PD-FL¹⁰ on the protein (Kovacev-Nikolic et al., 2016) and ModelNet10
 348 (Wu et al., 2015) datasets used previously in similar evaluations (Nishikawa et al., 2023). We also
 349 conduct an ablation study to compare PPM-FL with the unsupervised Rips filtration to demonstrate
 350 the effectiveness of PPM-FL. PPM-based approach can not use DTM since there are only $2q +$
 351 2 points in each random subset. In addition, we validate the robustness and scalability of PPM-
 352 FL. **In summary, while both PPM-FL and PD-FL produce comparable results in point cloud**
 353 **classification task, PPM-FL is more robust to outliers and has better scalability than PD-FL.**

354 All the classification results are obtained through 3-fold cross validation. All the experi-
 355 ments are conducted on a Ubuntu 20.04 system with 2TB RAM, AMD EPYC 7763 64-Core
 356 1500 MHZ CPU and NVIDIA A6000 GPU. The network is implemented with PyTorch 2.0.1.
 357 The code implementation of PD-FL is from <https://github.com/git-westriver/FiltrationLearningForPointClouds>. The details of the experiment setting are pro-
 358 vided in Appendix C. Code is provided at <https://anonymous.4open.science/r/PPM-FL-415C>.

362 6.1 COMPARISON WITH PD-FL

364 Following the same setting in Nishikawa et al. (2023) on the protein dataset, we employ the pipeline
 365 shown in Figure 1 with filtration learning, which uses the topological information only for classifi-
 366 cation. The results are shown in Table 2. The accuracies of PPM-FL over different homology di-
 367 mensions are significantly higher than PPM-Rips¹¹ and the standard deviation of PPM-FL is lower.

368 ⁹Hausdorff measure is a generalization of the traditional notions of area and volume to non-integer
 369 dimensions. Let k be a non-negative integer. For $A \subset \mathcal{M}$, and $\delta > 0$, consider $H_k^\delta(A) =$
 370 $\inf\{\sum_i \alpha(k) (\frac{\text{diam}(U_i)}{2})^k, A \subset \bigcup_i U_i \text{ and } \text{diam}(U_i) < \delta\}$, where $\alpha(k)$ is the volume of the k -dimensional
 371 unit ball and diam represents diameter. The k -dimensional Hausdorff measure on \mathcal{M} of A is defined by
 372 $H_k(A) = \lim_{\delta \rightarrow 0} H_k^\delta(A)$.

373 ¹⁰Here PD-FL means the PD-based Filtration Learning (Nishikawa et al., 2023). The experiments on com-
 374 paring PD-based filtration learning (PD-FL) with Rips (PD-Rips) and DTM (PD-DTM) filtration for PD have
 375 already been conducted in Nishikawa et al. (2023). PD-Rips produces similar results to that of PD-DTM. And
 376 PD-FL outperforms PD-Rips and PD-DTM. Hence, we just use PD-FL as baseline in our work.

377 ¹¹In the original PD-FL work (Nishikawa et al., 2023), it has been demonstrated that the Rips and DTM yield
 comparable results when applied to both the protein and the ModelNet10 dataset. For the sake of simplicity
 and to streamline our analysis, we will solely compare our proposed method with Rips.

378 This comparison with PPM-Rips demonstrates the advantage of the supervised filtration learning
 379 over the unsupervised filtration like Rips.
 380

381 Table 2: Accuracy of the binary classification task of protein structure. We compared our method
 382 PPM-FL with PPM-Rips and PD-FL. PPM-Rips denotes using the Rips filtration instead of the fil-
 383 tration learning for PPM. The PersLay vectorization is learned in an end-to-end way. Homology di-
 384 mension q stands for the dimension of PDs (PPMs). $q = 0\&1$ means that we use both 0-dimensional
 385 and 1-dimensional PD or PPM, and the feature input to the MLP is the concatenation of the vector-
 386 ization of 0-dimensional and 1-dimensional PDs (PPMs) via PersLay.
 387

	$q = 0$	$q = 1$	$q = 0\&1$
PD-FL	65.80 ± 1.76	82.10 ± 1.66	81.70 ± 1.31
PPM-Rips	64.09 ± 7.78	65.40 ± 2.12	71.50 ± 1.31
PPM-FL	84.00 ± 1.39	80.20 ± 1.76	84.60 ± 1.22

393 When compared with PD-FL, PPM-FL produces better results in $q = 0$ and $q = 0\&1$, but slightly
 394 worse in $q = 1$. This suggests that although PPM is a rather vague statistical approximation of PD,
 395 both of them are effective in extracting meaningful topological features from the protein dataset for
 396 classification. This could imply that the key aspect for achieving good performance in this context
 397 is not solely the precise topological information but rather the ability to appropriately integrate
 398 topological information with the classification model.
 399

400 For the ModelNet10 dataset, we use the version which contains 10 classes, with 100 instances in
 401 each class. Each instance is a point cloud of shape 128×3 . Here we employ the same two-phase
 402 process in Nishikawa et al. (2023) by combining topological embedding with a DNN-based method.
 403 For a point cloud X , let $\Psi_{\text{topo}}(X) \in \mathbb{R}^{L_1}$ be the topological embeddings from PD-FL or PPM-FL,
 404 $\Psi_{\text{DNN}}(X) \in \mathbb{R}^{L_2}$ be the feature from a DNN-based method. Let ℓ be the loss function and m be
 405 the number of classes. The two-phase training classifiers proposed by Nishikawa et al. (2023) are
 406 specified as follows:
 407

1. Phase 1 classifier receives feature from Ψ_{DNN} as $C_1 : \mathbb{R}^{L_2} \rightarrow \mathbb{R}^m$, where m is the number of
 408 classes. C_1 and Ψ_{DNN} are jointly learned by minimizing $\sum_j \ell(C_1(\Psi_{\text{DNN}}(X_j), y_j))$.
 409
2. Phase 2 classifier $C_2 : \mathbb{R}^{L_1+L_2} \rightarrow \mathbb{R}^m$. We fix the parameters of the learned Ψ_{DNN} in the 1st
 410 phase and learn C_2 and Ψ_{topo} by minimizing $\sum_j \ell(C_2([\Psi_{\text{DNN}}(X_j)^\top, \Psi_{\text{topo}}(X_j)^\top]^\top), y_j)$.
 411

412 The final classification is conducted through C_2 with the concatenated features from Ψ_{DNN} and
 413 Ψ_{topo} on the test set. For the choices of DNN method, we consider DeepSets (Zaheer et al., 2017),
 414 PointNet (Qi et al., 2017) and PointMLP (Ma et al., 2022). The results of the two-phase process are
 415 shown in Table 3.
 416

417 Table 3: Accuracies for the classification task on the ModelNet10 dataset. Two-phase training
 418 process is utilized here. The first phase we use DeepSets and PointNet. The results of PointMLP are
 419 discussed in Appendix D.1. The first phase directly uses point cloud as input and does not have the
 420 notion of homology dimension since it does not involve topological summary like PD or PPM. So
 421 there is no result for each homology dimension in the first phase.
 422

1st Phase		2nd Phase		
		PD-FL	PPM-Rips	PPM-FL
DeepSets 66.23 ± 3.19	$q = 0$	67.40 ± 2.31	67.30 ± 2.41	67.90 ± 3.01
	$q = 1$	68.20 ± 2.37	67.50 ± 2.17	66.90 ± 2.17
	$q = 0\&1$	67.40 ± 0.82	67.10 ± 1.42	67.50 ± 2.88
PointNet 67.23 ± 1.80	$q = 0$	68.60 ± 3.09	67.10 ± 2.21	68.70 ± 2.23
	$q = 1$	68.90 ± 2.64	67.10 ± 2.21	69.60 ± 1.33
	$q = 0\&1$	69.00 ± 5.57	67.30 ± 2.02	69.80 ± 0.77

When using DeepSets in the first phase, PD-FL, PPM-Rips and PPM-FL can all improve the classification accuracy in the second phase. Except for the case of $q = 1$ where PD-FL outperforms PPM-Rips and PPM-FL, PPM-FL achieves comparable results with PD-FL and PPM-Rips. This demonstrates the effectiveness of topological info when combined with the DNN method.

When using PointNet in the first phase, PPM-Rips makes no improvement on the classification accuracy. PPM-FL produces comparable results to that of PD-FL: both of them improve the accuracy in the second phase. The highest accuracy (69.80 ± 0.77) is obtained via PointNet + PPM-FL with homology dimensions $q = 0\&1$.

The additional results of PointMLP are discussed in Appendix D.1. The ablation study of the Gaussian weight is provided in Appendix D.3. Table 8 shows the effectiveness of our proposed Gaussian weight: by prioritizing nearer subsets, the Gaussian weight effectively amplifies meaningful topological features, thereby enhancing the method’s performance in capturing the intrinsic structure of the data.

It is worth noting that using all the homology dimensions is a rather safe choice to get high accuracy. Hence we will use all the homology dimensions in the following experiments.

6.2 ROBUSTNESS

Here we show the robustness of PPM against outliers in the point cloud. For the ModelNet10 dataset, we use the model trained on outlier-free point clouds; and for each point cloud in the test set, we add outliers from uniform distribution at percentage ϵ . We choose the two-phase process where the first phase uses DeepSets and the second phase uses all the homology dimensions $q = 0\&1$, since in this case PPM-FL and PD-FL produces similar results when there is no outliers on the test set, ensuring a fair comparison.

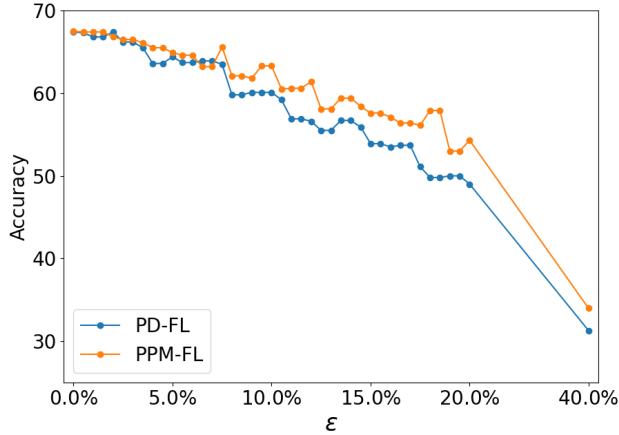


Figure 3: Average classification accuracy under different outlier percentages (ϵ). [The actual accuracies, corresponding standard deviations and analysis are provided in Appendix D.5.](#)

The average accuracies of PPM-FL and PD-FL under different outlier percentages ϵ are shown in Figure 3. PPM-FL and PD-FL produce similar results when the number of outliers is small, i.e., $\epsilon \leq 5.0\%$. When the number of outliers increases, i.e., $\epsilon > 5.0\%$, the accuracy of PD-FL drops quickly while PPM-FL remains accuracy above 55% when $\epsilon \leq 18.5\%$. This result validates the robustness against outliers of PPM shown in Section 5.

6.3 SCALABILITY W.R.T. POINT CLOUD SIZE

We demonstrate the scalability of PPM-FL w.r.t. the point cloud size n . The settings in each phase here are the same as that in last subsection on robustness. The number of the point clouds in the dataset is fixed. We consider both homology dimensions 0 and 1 in the second phase. We fix the batch size and report the average time of each epoch in the second phase in Table 4. In the first phase, we use the same pretrained model for PPM-FL and PD-FL.

486
 487 Table 4: Actual time cost (s) per-epoch under different numbers n of points in the point cloud
 488 and numbers of random subsets M in PPM. Our aim is to compare the real-world usage of these
 489 methods on the ModelNet10 dataset. Thus, PPM-FL is conducted on GPU and PD-FL is on pure
 490 CPU or CPU-GPU Hybrid. The computation of PD-FL (CPU) is through the GUDHI library (Maria
 491 et al., 2014). The computation of PD-FL (CPU-GPU Hybrid) is through the *torch-topological* library
 (AIDOS-Lab).

	PPM-FL (GPU)			PD-FL (CPU)	PD-FL (Hybrid)
	M=100	M=200	M=400		
n=64	56.61 \pm 1.08	112.79 \pm 1.41	210.17 \pm 2.50	41.46 \pm 2.55	5.59 \pm 0.23
n=128	58.91 \pm 3.11	118.79 \pm 1.22	218.26 \pm 1.35	187.56 \pm 2.87	29.46 \pm 2.42
n=256	65.85 \pm 1.04	129.19 \pm 1.15	239.42 \pm 1.01	1101.85 \pm 11.46	157.95 \pm 1.95
n=512	77.95 \pm 1.77	154.32 \pm 1.58	273.47 \pm 1.26	7556.32 \pm 66.11	607.95 \pm 13.20

500
 501 For PPM-FL, when the number of random subsets M is fixed, the time cost increases very modestly
 502 as n grows. When the number of points in each point cloud n is fixed, the time cost is linear w.r.t.
 503 M .

504 Compared with PD-FL (CPU), PPM-FL’s time cost is similar to that of PD-FL (CPU) when point
 505 cloud size n is very small. PD-LF (Hybrid) is one order of magnitude faster than PD-FL (CPU).
 506 But when n is very large ($n \geq 512$), PD-LF (Hybrid) is slower than PPM-FL (GPU). The time
 507 cost of PD-FL, whether on CPU or hybrid, increases very rapidly when n grows. This demonstrates
 508 PPM-FL possesses better scalability than PD-FL.

509
 510 Table 5: Accuracies of PPM-FL (GPU) under different M s ($n = 128, q = 0\&1$) on the ModelNet10
 511 dataset with the 1st phase model being DeepSets.

$M = 25$	$M = 50$	$M = 100$	$M = 200$	$M = 400$
67.00 \pm 2.53	67.00 \pm 1.43	67.60 \pm 2.20	67.50 \pm 2.88	67.40 \pm 1.92

516
 517 Table 6: Accuracies of PPM-FL (GPU) under different n s ($M = 100, q = 0\&1$) on the ModelNet10
 518 dataset with the 1st phase model being DeepSets.

$n = 128$	$n = 256$	$n = 512$
67.60 \pm 2.20	71.65 \pm 1.84	69.40 \pm 2.94

523 Some selected accuracy results corresponding to Table 4 are shown in Table 5 and 6. These results
 524 explicitly demonstrate that scalability of PPM-FL is achieved without sacrificing accuracy. And
 525 according to Table 5, empirically, if $M(2q + 2)$ is close to or smaller than n , i.e. only a small subset
 526 of the entire point cloud is sampled, the performance of PPM-FL will degrade. Hence, a default
 527 choice of M would be an integer larger than $n/(2q + 2)$.

528 7 CONCLUSION

531 In this study, we propose to use PPM to replace PD in a filtration learning framework. PPM-based
 532 filtration learning (PPM-FL) addresses the scalability limitations of existing PD-based approach for
 533 point clouds. By leveraging PPM, which can be computed entirely on GPU in a parallel manner, we
 534 achieved a more efficient solution for encoding topological features.

535 Our theoretical analysis establishes the robustness of PPM against outliers, and we experimentally
 536 validate this property in the context of supervised filtration methods. The results show that PPM-
 537 FL maintains more stable performance than PD-FL when the test point cloud is contaminated with
 538 outliers.

539 Limitation and future works are discussed in Appendix D.6.

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702

A BACKGROUND

703

A.1 EXPECTED PERSISTENCE DIAGRAM

706 A PD $\mathcal{D} = \{r_i = (b_i, d_i) \in \Omega | 1 \leq i \leq N(\mathcal{D})\}$ can be equivalently represented as a counting
 707 measure μ on Ω given by $A \in \mathcal{B} \rightarrow \mu(A) = \sum_{i=1}^{N(\mathcal{D})} \delta_{r_i}(A)$,

708 where \mathcal{B} is the class of all Borel subsets of Ω and δ_r denotes the Dirac point mass at $r \in \Omega$. When
 709 each sampled PD is a random draw from a distribution P , its EPD, denoted as $\mathbb{E}[\mu]$, is defined as
 710 $A \in \mathcal{B} \rightarrow \mathbb{E}[\mu](A) = \mathbb{E}[\mu(A)]$ (Chazal & Divol, 2018).

712 Given a finite set $\{\mu_1, \mu_2, \dots, \mu_n\}$, consisting of sampled PDs from P , the empirical EPD is defined
 713 as $\bar{\mu} = \frac{1}{n} \sum_{i=1}^n \mu_i$. The support of $\bar{\mu}$ is $\mathcal{S}_{\bar{\mu}} = \bigcup_{i=1}^n \mathcal{D}_i$, where $\mathcal{D}_i = \{r_j = (b_j, d_j) \in \Omega | 1 \leq j \leq$
 714 $N(\mathcal{D}_i)\}$ is the support of the sampled PD μ_i . EPD can be viewed as a distribution (Chazal & Divol,
 715 2018) of topological features supported on the open half plane Ω . Quantization method (Divol &
 716 Lacombe, 2021a) has been developed to reduce the support size of EPD.

717 An inherent metric applicable to the space of EPDs (Divol & Lacombe, 2021a) with the same mass,
 718 is Wasserstein distance (Villani, 2009). In a space of EPDs with different masses, the Optimal
 719 Partial Transport metric (OT_p) (Figalli, 2010) is used to allow any mass transportation from or to the
 720 diagonal $\partial\Omega$.

721 For the approximation error of EPD, we have the following theorem in Cao & Monod (2022):

722 **Theorem A.1** (Cao & Monod (2022)). *Let $X \subset \mathbb{R}^m$ be a finite set of points, and π be a probability
 723 measure on X satisfying the (a, b, r_0) -standard assumption. Suppose X_s^1, \dots, X_s^M are M i.i.d.
 724 samples from the distribution $\pi^{\otimes n}$ with $|X_s^i| = n$. Let $\bar{\mu}$ be the empirical persistence measure, i.e.,
 725 EPD; denote $\beta := \frac{p}{b} - 1$. Then the empirical persistence measure approaches the true persistence
 726 measure $\mathcal{D}(X)$ (here we omit the symbol filtration choice and $\mathcal{D}(X)$ is in measure form: $\mathcal{D}(X) =$
 727 $\sum_r \delta_r$) of X in expectation at the following rates:*

$$\mathbb{E}[\text{OT}_p^p(\bar{\mu}, \mathcal{D}(X))] \leq \begin{cases} O(M^{-1/2}) + O(1) + O(n^{-\beta}) & \text{if } p > b; \\ O(M^{-1/2}) + O(1) + O\left(\left(\frac{\log n}{n}\right)^{1/b}\right) & \text{if } p \leq b, r_0 < \left(\frac{\log n}{an}\right)^{1/b}; \\ O(M^{-1/2}) + O(1) + O\left(\left(\frac{\log n}{n}\right)^{p/b} \frac{1}{(\log n)^2}\right) & \text{if } p \leq b, r_0 \geq \left(\frac{\log n}{an}\right)^{1/b}. \end{cases}$$

734

A.2 PRINCIPAL PERSISTENCE MEASURE

736 As a special case of Expected Persistence Diagram, the approximation error and convergence analysis
 737 of the empirical measure to Principal Persistence Measure is theoretically studied in Theorem
 738 3.20 in Gómez & Mémoli (2024): the empirical measure converges to PPM almost surely as the
 739 number of subsets $M \rightarrow \infty$.

740 For the stability of PPM, we have the following Theorem A.2 from Tung et al. (2025).

743 **Theorem A.2** (Tung et al. (2025)). *Let $p \geq 1$, and let W_p denote the p -Wasserstein metric on \mathbb{R}^d
 744 and Ω' . A key property shown in Gómez & Mémoli (2024) Theorem 3.8, Theorem 4.11 is that PPMs
 745 are stable:*

$$W_p(\text{PPM}_q(\mu), \text{PPM}_q(\nu)) \leq C_q W_q(\mu, \nu),$$

747 for all $\mu, \nu \in \mathcal{P}_c(\mathbb{R}^d)$, where $C_q > 0$ is a constant which depends on homology dimension q and
 748 $\mathcal{P}_c(\mathbb{R}^d)$ is the Borel probability measure with compact support on \mathbb{R}^d .

750 The $\text{PPM}_q(\mu)$ here means the Principal Persistence Measure with homology dimension q computed
 751 from points sampled from measure μ supported on \mathbb{R}^n and the PPM is transformed from the (birth,
 752 death) to (birth, persistence) space $\Omega' = \{(b, l) \in \mathbb{R}^2\} \setminus \{l = 0\}$, where persistence=death-birth ≥ 0 .
 753 This is a slightly rotated version of the PPM we considered in the $\Omega = \{(t_1, t_2) \in \mathbb{R}^2 | t_2 > t_1\}$.

754 For the computation of PPM, we have the following theorem:

755 **Theorem A.3** (Gómez & Mémoli (2024)). *Let (X, d_X) be a metric space with n points. Then:*

756 1. For all homology dimension larger than $\frac{n}{2} - 1$, the PD obtained via Rips filtration is empty.
 757
 758 2. If n is even and homology dimension equals to $\frac{n}{2} - 1$, then the PD obtained via Rips filtration
 759 consists of a single point $r_1 = (t_b, t_d)$ if and only if $t_b < t_d$, and is empty otherwise.
 760

761 A.3 NOTES ON DEATH TIME
 762

763 Death times are finite when the homology dimension is zero and this results a point $r = (0, \infty)$ in
 764 the PD, representing the final connected component. In practice, for vectorization, we usually set
 765 the maximum threshold for the filtration to be a finite value or just remove the point with infinite
 766 death time since it exists for all point clouds and has no practical value. So here we focus on the
 767 practice aspect and assume the death time is always finite. We ignore the topological feature with
 768 infinite death time.
 769

770 A.4 VECTORIZATION VIA PERSLAY
 771

772 PersLay (Carrière et al., 2020) is a supervised vectorization method for PD, a multiset $\mathcal{D} = \{r_i =$
 773 $(b_i, d_i) \in \Omega | 1 \leq i \leq N(\mathcal{D})\}$ on the half plane $\Omega = \{(t_1, t_2) \in \mathbb{R}^2 | t_2 > t_1\}$. PersLay is adapted
 774 from the DeepSets structure (Zaheer et al., 2017) and expressed as follows:
 775

$$\text{PersLay}(\mathcal{D}) = \mathbf{op}(\{w(r) \cdot \phi(r)\}_{r \in \mathcal{D}}),$$

776 where \mathbf{op} is any permutation invariant operation (such as minimum, maximum, sum, kth largest
 777 value...), $w : \mathbb{R}^2 \rightarrow \mathbb{R}$ is a weight function for the points in PD, and $\phi : \mathbb{R}^2 \rightarrow \mathbb{R}^q$ is a representation
 778 function called point transformation, mapping each point (b_i, d_i) of a PD to a vector.
 779

780 Certain choices of w , ϕ and \mathbf{op} can transform PersLay into specific methods like Persistence Image
 781 (Adams et al., 2017) and Persistence Landscape (Bubenik et al., 2015). In our work, we follow the
 782 setting in Nishikawa et al. (2023) and choose $w(\cdot) = 1$ and ϕ as
 783

$$\phi(r) = [\exp(-\frac{\|p - c_1\|^2}{2}), \exp(-\frac{\|p - c_2\|^2}{2}), \dots, \exp(-\frac{\|p - c_m\|^2}{2})]^\top,$$

784 where $r = (b, d)$, $p = (b, d - b)$ and all the c_i s are the parameters to be learned.
 785

786 **Non-DL vectorization.** While our current work is more centered on the scalability of our proposed
 787 method within the DL-based context, we recognize the importance of the non-DL perspective. Re-
 788 garding the non-DL based vectorization method, the scalability issue of Expected Persistence Dia-
 789 gram (EPD), a more general form of PPM, has been discussed in detail in Bubenik et al. (2015) and
 790 Section 4.3.1 in Gómez & Mémoli (2024).
 791

792 A.5 PERSISTENCE DIAGRAM-BASED FILTRATION LEARNING FRAMEWORK
 793

794 The PD-based filtration learning framework (PD-FL) (Nishikawa et al., 2023) is shown in Figure
 795 4. PD-FL tries to learn the weight function $w(\cdot) = f_\theta(X, \cdot)$ from the entire point cloud X for
 796 weighted filtration. Once the weight is learned, weighted filtration is used to compute PD. Then, PD
 797 is vectorized by PersLay and used in machine learning task like point cloud classification.
 798

799 B PROOF AND RELATED ANALYSIS
 800

801 B.1 ON THE ASSUMPTION OF P AND U IN LEMMA 5.1 & THEOREM 5.2
 802

803 We have the following two assumptions on P and U .
 804

1. We assume that P and U share the same support. Regarding the manifold's support, U
 805 is a (maybe uniform) distribution over the entire support of \mathcal{M} , including regions where
 806 the inlier density P are very low and points have little chance to be sampled from this low
 807 density area. An example is shown in Figure 16 in Gómez & Mémoli (2024). The support
 808 of P is the circular area and the low density region lies at the inner part of the ring.
 809
2. P and U are both lower and upper bounded in the support, i.e. there exist constants $\bar{c} \geq$
 $\underline{c} > 0$ such that $\bar{c} \geq P(x) \geq \underline{c}$ and $\bar{c} \geq U(x) \geq \underline{c}$ for any x in the support.
 810

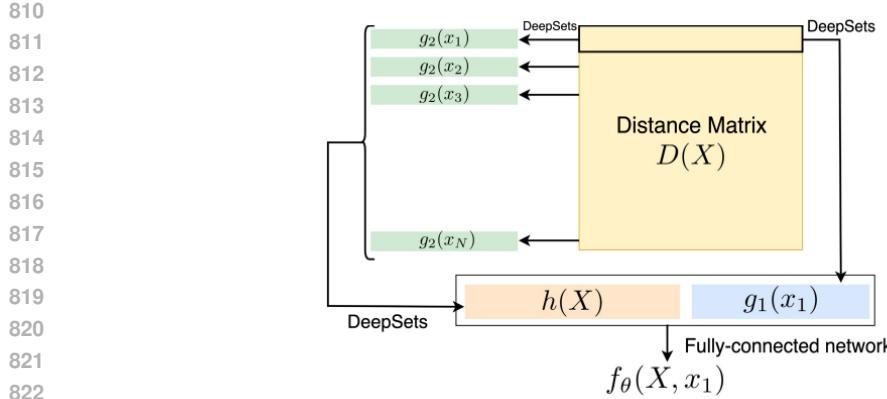


Figure 4: Persistence Diagram-based Filtration Learning Framework. Functions g_1 , g_2 and h are the same as those we use in Section 4. This is a direct reuse of Figure 2 in Nishikawa et al. (2023).

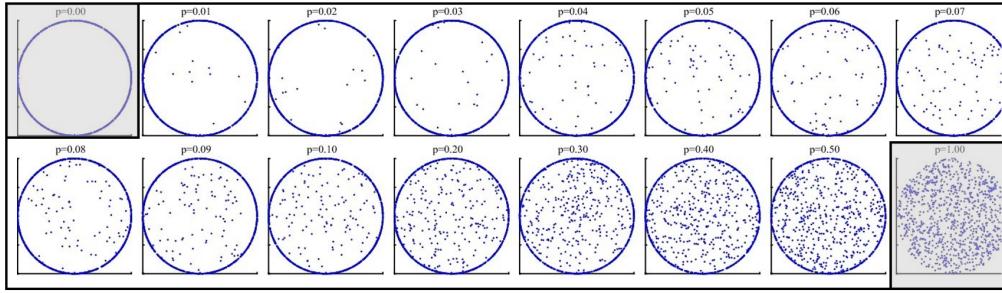


Figure 5: Part of Figure 16 from Gómez & Mémoli (2024).

The caption of Figure 16 in Gómez & Mémoli (2024) claims that "Given $0 \leq p \leq 1$, we sample $X \subset D^2$ with 1000 points so that each point is uniformly distributed in the interior of D^2 with probability p or on its boundary \mathbb{S}_E^1 with probability $1-p$ ". We can consider P is such a distribution with a p that is close to 0, but it is not 0. And consider U is a distribution with p that is close to 1, but it is not 1. So both the supports of P and U are $D^2 \cup \mathbb{S}_E^1$ and the value of their pdf is upper and lower bounded. And it would not cause the pdf being either 0 or infinite, as shown in the area not shaded in Figure 5. This aligns with our assumptions above.

B.2 PROOF OF LEMMA 5.1

Lemma 5.1. For EPD $\mathbb{E}_{X_s \sim P^n}[\nu(X_s)]$ with density μ_1 and $\mathbb{E}_{X_s \sim P_o^n}[\nu(X_s)]$ with density μ_2 , where $\nu(X_s)$ is the measure form of PD $\mathcal{D}(\mathcal{K}(X_s))$, i.e., $\nu(X_s) = \sum_{r \in \mathcal{D}(\mathcal{K}(X_s))} \delta_r$, it holds that

$$\|\mu_1 - \mu_2\|_1 \leq C_n H_k(\mathcal{M})^n p_{n-1}(\epsilon) \epsilon,$$

where C_n is the expected number of points in the PD built with the filtration \mathcal{K} on n i.i.d. uniform points on \mathcal{M} , $H_k(\mathcal{M})$ is k -dimensional Hausdorff measure of \mathcal{M} and $p_{n-1}(\epsilon)$ is a polynomial of order $n-1$ with bounded coefficients.

Proof. For Theorem 7.1 in Chazal & Divol (2018), we have that

$$\|\mu_1 - \mu_2\|_1 \leq C_n H_k(\mathcal{M})^n \|q_1 - q_2\|_\infty,$$

where $q_1(q_2)$ is the density with respect to the Hausdorff measure H_k , $q_1(x) = \Pi_{i=1}^n P(x_i)$ and $q_2(x) = \Pi_{i=1}^n P_o(x_i)$, where $x = [x_1^\top, \dots, x_n^\top]^\top$. For the $\|q_1 - q_2\|_\infty$ term, since each x_i is i.i.d. sampled, for $x = \text{argmax}|q_1 - q_2|$, it holds that

$$\begin{aligned}
 (q_1 - q_2)(x) &= \Pi_i P(x_i) - \Pi_i P_o(x_i) \\
 &= \Pi_i P(x_i) \left[1 - \frac{\Pi_i P_o(x_i)}{\Pi_i P(x_i)} \right],
 \end{aligned}$$

864 where under the assumption that each x_i is in the support (with positive density) of P and $1 >$
 865 $\frac{U(x_i)}{P(x_i)} \geq \Delta > 0$, we have that
 866

$$\begin{aligned} \frac{\Pi_i P_o(x_i)}{\Pi_i P(x_i)} &= \Pi_i [1 - (1 - \frac{U(x_i)}{P(x_i)})\epsilon] \\ &\geq \Pi_i [1 - (1 - \Delta)\epsilon] \end{aligned}$$

870 So it holds that

$$\begin{aligned} \|q_1 - q_2\|_\infty &= |q_1(x) - q_2(x)| \\ &\leq \Pi_i P(x_i) [1 - (1 - (1 - \Delta)\epsilon)^n] \\ &= p_{n-1}(\epsilon)\epsilon. \end{aligned}$$

875 Finally, we obtain that

$$\| \mu_1 - \mu_2 \|_1 \leq C_n H_k(\mathcal{M})^n p_{n-1}(\epsilon)\epsilon.$$

877 \square

879 B.3 THE DEPENDENCE ON OUTLIER DISTRIBUTION U

880 The upper bound in Lemma 5.1 is dependent on U . This dependence is reflected in the coefficients
 881 of the polynomial $p_{n-1}(\epsilon)$. As shown in the proof above, the polynomial's coefficients are derived
 882 from $\Delta = \inf \frac{U(x)}{P(x)}$ (the minimum ratio of outlier to inlier densities over \mathcal{M}), which is dependent on
 883 noise U .

884 For the area where P is dense and U is sparse, a sparser U will result a small Δ . This will lead to
 885 smaller absolute values of the coefficients in the polynomial $p_{n-1}(\epsilon)$, i.e. a smaller upper bound.
 886 This corresponds to the intuition that EPD (or PPM) is more robust to a sparser outlier distribution.

890 C EXPERIMENT SETTINGS

891 **Optimization.** We set the batch size as 128 for protein datasets and 40 for ModelNet10
 892 dataset. For optimizer, we use Adam. Learning rate is 0.1 for ModelNet and 0.001 for
 893 protein dataset. For scheduler, we use the TransformerLRScheduler implemented in pytorch
 894 (<https://github.com/sooflware/pytorch-lr-scheduler/tree/main>) and the
 895 number of warm-up epoch is set to be 40. For ModelNet10, the number of epochs in
 896 the first phase is 1500. For protein dataset and the second phase of ModelNet dataset, we
 897 use the EarlyStopping handler (https://pytorch.org/ignite/generated/ignite.handlers.early_stopping.EarlyStopping.html) with patience=20 and min_delta =
 898 0.002 for the loss on validation set of size 200.

899 **Principal Persistence Measure.** For the computation of PPM, we set $M = 200$ for both protein
 900 and ModelNet10 datasets. For the vectorization method PersLay, the length of vectorization m is
 901 set to be 32 and the permutation invariant operation **op** is summation.

902 **Networks.** For the DNN-based methods (DeepSets, PointNet and PointMLP) in the first phase, we
 903 use the same structure as those in Nishikawa et al. (2023). We set all of the permutation invariant
 904 operators **op** that appear in PPM-FL and PD-FL are all summation. The dimension of the feature
 905 vectors obtained by PersLay is set as 16, except that when using both homology dimensions, it is
 906 32. The DeepSets-like structures $\phi^{(1)} - \phi^{(5)}$ and fully connected network are the same as those in
 907 Nishikawa et al. (2023). We initialized the parameters in PPM-FL with normal distribution with a
 908 mean of 0 and a standard deviation of 1.0. Other parameters were initialized with the default settings
 909 of PyTorch.

910 **Datasets.** The protein dataset (Kovacev-Nikolic et al., 2016) does not provide a point cloud. Instead,
 911 a cross-correlation matrix \mathbb{C} is provided for each protein. Then the dynamic distance matrix \mathbb{D} ,
 912 where $\mathbb{D}_{i,j} = 1 - |\mathbb{C}_{i,j}|$, is used to compute PD or PPM. We use a version of this dataset (Nishikawa
 913 et al., 2023), which contains two classes of protein, with 500 instances in each class. Each instance is
 914 a distance matrix of shape 60×60 and has noise from a uniform distribution with standard deviation
 915 of 0.1 for the off-diagonal elements. For the ModelNet10 dataset, we use the version which contains
 916 10 classes, with 100 instances in each class. Each instance is a point cloud of shape 128×3 .

918 D ADDITIONAL RESULTS AND DISCUSSIONS

919 D.1 RESULTS OF TWO-PHASE TRAINING (POINTMLP + PPM-FL)

920 For PointMLP, it is claimed in Nishikawa et al. (2023) that PD-FL reduces the accuracy of 68.80 to
 921 below or around 60 in the first phase, because PointMLP has already captured information including
 922 topology in the first phase and PD-FL brings in redundant information.

923 Table 7: Accuracie for the classification task of ModelNet10 dataset when the first phase is
 924 PointMLP.

925 1st Phase	926 PointMLP	927 70.10 ± 4.70		
928 2nd Phase	929 PPM-Rips 930 PPM-FL	$q = 0$ 931 54.20 ± 9.56	$q = 1$ 932 57.30 ± 13.37	$q = 0\&1$ 933 49.29 ± 11.82
		52.70 ± 8.58	53.90 ± 8.23	56.59 ± 13.01

934 The results of the two-phase process where the first phase uses PointMLP are shown in Table 7.
 935 Despite the choice of homology dimension, the accuracy of PPM-FL in the second phase is signif-
 936 icantly lower than that in the first phase. This confirms the claim in Nishikawa et al. (2023) that
 937 PointMLP has already captured information including topology in the first phase and PD-FL brings
 938 in redundant information.

939 At a higher level, the topological information here is specific pairwise distance that is topologically
 940 meaningful, since the birth and death of a topological feature in PD or PPM are actually pairwise
 941 distances. In PointNet and DeepSets, no pairwise information is needed because both of them use a
 942 network to transform point feature and then use a permutation invariant operator to aggregate these
 943 features as point cloud-level feature. But PointMLP needs pairwise info to define a neighborhood
 944 in order to learn the feature of a local region. This process involves pairwise distances. This could
 945 explain why PPM or PD can only work for PointNet and DeepSets, rather than PointMLP.

946 D.2 RELATION BETWEEN PPM AND THE DISTRIBUTION OF PAIRWISE DISTANCES.

947 It is worth mentioning that when homology dimension $q = 0$ and we use the unsupervised Rips
 948 filtration instead of the filtration learning, PPM represents the distribution of pairwise distances,
 949 which is shown in Boutin & Kemper (2005) to almost solve the isometry classification problem for
 950 point clouds. PPM of higher homology dimension can be viewed as a conditional distribution of
 951 pairwise distances that are topologically meaningful for high dimensional cycles.

952 D.3 ABLATION STUDY ON WEIGHT CHOICE: GAUSSIAN OR UNIFORM

953 We present supplementary experimental results of PPM-FL with Gaussian ($\sum_{i=1}^M K(X_s^i) f(X_s^i, \cdot)$)
 954 or Uniform ($\sum_{i=1}^M f(X_s^i, \cdot)$) weight on the ModelNet10 dataset, under the same setting as that in
 955 Table 3. In the first phase, we use DeepSets. The results are shown in Table 8. For the choice of K
 956 , any differentiable distributional kernel would be fine. For simplicity, we choose to use Gaussian
 957 Distribution Kernel. The hyperparameter σ is set to be the median of all the pairwise distances. Our
 958 current results demonstrate effectiveness with this default setting.

959 Table 8: Accuracies of PPM-FL on ModelNet10 dataset under different weight functions.

	$q = 0$	$q = 1$	$q = 0\&1$
Gaussian	67.90 ± 3.01	66.90 ± 2.17	67.50 ± 2.88
Uniform	67.60 ± 1.97	67.00 ± 2.21	66.80 ± 1.87

960 In our pipeline, the first phase uses DeepSets, while the second phase employs PPM-FL with either
 961 a Gaussian or Uniform weight function. As demonstrated in the table below, across different ho-
 962 mology dimensions, PPM-FL utilizing the Gaussian weight either outperforms or achieves similar
 963 results with the Uniform weight variant. This outcome validates the effectiveness of the Gaussian

972 weight function, aligning with the design principle that subsets in closer proximity should have a
 973 more substantial influence. While the performance differences are subtle given the nature of the
 974 dataset, Table 8 shows the effectiveness of our proposed Gaussian weighting.
 975

976 D.4 RELATION BETWEEN THEOREM 5.2 AND EXISTING RESULTS IN DIVOL & LACOMBE 977 (2021b).

979 Here we discuss the difference between our theoretical results (Theorem 5.2) with the two Proposi-
 980 tions (5.4 & 5.5) in Section 5.3 of Divol & Lacombe (2021b).

- 981 • In Proposition 5.4, the support of distribution P and P' is \mathcal{M}^p , the space of PDs (measures)
 982 with finite persistence. Proposition 5.4 demonstrates that the expectation of P , i.e. EPD,
 983 is stable with respect to the distortion (P') of P . While our result is about the stability of
 984 EPD with respect to the addition of outliers of distribution P , which is supported on \mathbb{R}^d
 985 (instead of \mathcal{M}^p), the space where we sample the subsets.
- 986 • Proposition 5.5 demonstrates the stability of EPD with respect to the distribution ξ sup-
 987 ported on \mathbb{R}^d . This is similar to our result in Lemma 5.1, with $P(P_o)$ corresponding to
 988 $\xi(\xi')$. Compared with Proposition 5.5, our result (Lemma 5.1) takes a specific form of
 989 $P_o = (1 - \epsilon) \cdot P + \epsilon \cdot U$ (a mixture of the original distribution P and outlier distribution
 990 U) and links the upper bound to the mixture proportion ϵ , while Proposition 5.5 generally
 991 gives the upper bound as the bottleneck distance $W_\infty(\xi, \xi')$. It could be argued that our
 992 result is a specific case of Proposition 5.5 of Divol & Lacombe (2021b).

994 D.5 RESULTS UNDER DIFFERENT OUTLIER PERCENTAGES

996 Table 9: **Accuracies and standard deviations under different outlier percentages (ϵ s).** The first phase
 997 uses DeepSets. The second phase uses both homology dimensions $q = 0\&1$.

ϵ	PPM-FL	PD-FL	ϵ	PPM-FL	PD-FL
0.0%	67.50 ± 2.88	67.40 ± 0.82	10.5%	60.50 ± 1.16	59.20 ± 2.81
0.5%	67.40 ± 2.94	67.30 ± 0.29	11.0%	60.60 ± 0.09	56.90 ± 1.65
1.0%	67.40 ± 2.13	66.80 ± 1.84	11.5%	60.60 ± 0.09	56.90 ± 1.65
1.5%	67.40 ± 2.13	66.80 ± 1.84	12.0%	61.40 ± 1.42	56.60 ± 1.42
2.0%	66.80 ± 2.55	67.40 ± 1.07	12.5%	58.10 ± 1.45	55.50 ± 2.16
2.5%	66.50 ± 1.25	66.20 ± 0.76	13.0%	58.10 ± 1.45	55.50 ± 2.16
3.0%	66.50 ± 1.25	66.20 ± 0.76	13.5%	59.40 ± 2.02	56.70 ± 1.59
3.5%	66.10 ± 1.76	65.50 ± 2.05	14.0%	59.40 ± 2.02	56.70 ± 1.59
4.0%	65.50 ± 2.22	63.60 ± 1.53	14.5%	58.40 ± 1.49	55.90 ± 2.53
4.5%	65.50 ± 2.22	63.60 ± 1.53	15.0%	57.60 ± 1.11	53.90 ± 2.66
5.0%	64.90 ± 1.16	64.40 ± 1.91	15.5%	57.60 ± 1.11	53.90 ± 2.66
5.5%	64.60 ± 0.90	63.70 ± 0.49	16.0%	57.10 ± 1.62	53.50 ± 3.36
6.0%	64.60 ± 0.90	63.70 ± 0.49	16.5%	56.40 ± 1.96	53.70 ± 2.02
6.5%	63.20 ± 0.61	63.90 ± 2.75	17.0%	56.40 ± 1.96	53.70 ± 2.02
7.0%	63.20 ± 0.61	63.90 ± 2.75	17.5%	56.10 ± 2.59	51.10 ± 2.94
7.5%	65.60 ± 1.03	63.50 ± 2.03	18.0%	57.90 ± 0.91	49.80 ± 4.12
8.0%	62.10 ± 0.57	59.80 ± 0.61	18.5%	57.90 ± 0.91	49.80 ± 4.12
8.5%	62.10 ± 0.57	59.80 ± 0.61	19.0%	53.00 ± 1.09	50.00 ± 3.09
9.0%	61.80 ± 2.09	60.10 ± 1.52	19.5%	53.00 ± 1.09	50.00 ± 3.09
9.5%	63.30 ± 1.15	60.10 ± 2.00	20.0%	54.30 ± 1.32	49.00 ± 3.79
10.0%	63.30 ± 1.15	60.10 ± 2.00	40.0%	34.00 ± 2.11	31.30 ± 5.91

1023 We report accuracies and standard deviations corresponding to Figure 3 in Table 9. Around $\epsilon = 0$,
 1024 the accuracies of PPM-FL and PD-FL drop with a similar rate. When $\epsilon \leq 1.5\%$, the accuracy of
 1025 PPM-FL almost remains the same while PD-FL drops from 67.40 to 66.80. This demonstrates that
 a few outliers have more impact on PD-FL than PPM-FL. PD-FL does not ignore the first outliers

1026 while PPM-FL does. The reason behind this may be that when the number of outliers are small, the
 1027 outliers have very little chance to be selected in a small subset. When $\epsilon = 40.0\%$, both PPM-FL and
 1028 PD-FL have very bad performance.
 1029

1030 D.6 LIMITATION AND FUTURE WORK.

1031
 1032 **Limitation.** The approximation nature of PPM may lead to the loss of some fine-grained topolog-
 1033 ical information. Future work could explore ways to enhance the representational power of PPM
 1034 while maintaining its computational efficiency. In addition, Theorem 5.2 on robustness has practical
 1035 limitations, as its dependence on q makes it weak for higher homology dimension. This leads to the
 1036 result that the fraction of noise has to be very small to control the measure errors. Our experimental
 1037 results in Figure 3 align with this: while PPM-FL is not highly robust, it degrades more gradu-
 1038 ally than PD-FL as outliers increase (maintaining accuracy above 55% when $18.5\% \geq \epsilon > 5\%$),
 1039 showing a modest improvement.
 1040

1041 **Future Work.** Further research could focus on extending the PPM-FL framework to more complex
 1042 point cloud tasks, such as 3D object reconstruction or semantic segmentation. In addition, as noted
 1043 in Nishikawa et al. (2023), learned weights are difficult to interpret. For PPM, due to the inherent
 1044 nature of subsampling, the interpretability of its learned weights is even lower. Developing methods
 1045 capable of learning far more interpretable weight functions will be part of our future work.
 1046

1047 E ON THE USE OF LARGE LANGUAGE MODELS

1048 Large Language Models (LLMs) were utilized in the polishing phase of this paper’s preparation.
 1049 Specifically, LLMs were employed to optimize linguistic clarity, enhance stylistic coherence, and
 1050 correct minor grammatical or syntactical inconsistencies. All core intellectual content, includ-
 1051 ing conceptual frameworks, empirical observations, argumentative structure, and citation align-
 1052 ment—was developed, curated, and validated exclusively by the human authors.
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