Randomly Pivoted V-optimal Design: Fast Data Selection under Low Intrinsic Dimension

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Abstract

Despite the ubiquitous high-dimensionalities brought about by the increasing sizes of models and data, low intrinsic dimensions are commonly found in many high-dimensional learning problems (e.g. finetuning). To explore sample efficient learning that leverages such low intrinsic dimensions, we introduce randomly pivoted V-optimal design (RPVopt), a fast data selection algorithm that combines dimension reduction via sketching and optimal experimental design. Given a large dataset with N samples in a high dimension d, RPVopt first reduces the dimensionality from d to $m \ll d$ by embedding the data to a random low-dimensional subspace via sketching. Then a coreset of size n > m is selected based on the low-dimensional sketched data through an efficient two-stage random pivoting algorithm. With a fast embedding matrix for sketching, RPVopt achieves an asymptotic complexity of O(Nd + Nnm), linear in the full data size, data dimension, and coreset size. With extensive experiments in both regression and classification settings, we demonstrate the empirical effectiveness of RPVopt in data selection for finetuning vision tasks.

1 Introduction

Deep learning models have achieved remarkable success across various domains, including vision [1, 2] and languages [3, 4]. These large models typically require training on astronomical-scale datasets [5, 6]. However, the computational costs and data storage demands associated with such datasets pose substantial challenges. Consequently, there is increasing interest in enhancing data efficiency and reducing dataset sizes without sacrificing performance. Prominent strategies such as coreset selection and data condensation have emerged. By identifying and retaining a condensed yet representative sample set from larger datasets, these techniques allow the training of models on smaller, yet representative, datasets that aim to mirror the learning potential of the full dataset.

Despite the increasing dimensionalities in modern machine learning, low intrinsic dimensions can often be found in many high-dimensional learning problems like finetuning [7, 8]. Inspired by this seminal work, there are follow-up works [9, 10] employing a low-dimensional reparameterization for parameter-efficient finetuning. Such low intrinsic dimensions suggest that, under suitable regularization, learning with a small subset of the huge original dataset should be sufficient to mimic the performance of full-size training. Recent work also shows that compressing the model via intrinsic

^{*}Alphabetical order.

dimension yields better results than standard pruning and uses them to derive compression-based generalization bounds [11].

For statistical models, data selection is often formulated as an optimal experimental design (OED) problem [12, 13, 14, 15]. In the classical overdetermined setting for OED (where the problem dimension d is lower than the data size n), V(ariance)-optimality is a design criterion tailored to control the generalization gap. Inspired by the recent progress [16] on extending the notion of V-optimality to overparametrized data selection with low intrinsic dimension via sketching, we introduce Randomly Pivoted V-optimal Design (RPVopt), a fast data selection method for learning under low intrinsic dimension.

Concretely, RPVopt first explores the low intrinsic dimension by embedding the high-dimensional problem to a random low-dimensional subspace via sketching [16]. After reducing to the classical low-dimensional (overdetermined) setting, in contrast to the common practice of solving an expensive continuous relaxation of the discrete optimization problem posed by V-optimality [17, 18, 16], we introduce a more efficient two-stage random pivoting algorithm that samples the coreset adaptively. For the full data size N, problem dimension d, coreset size n, and embedding dimension m, RPVopt runs in O(Nd + Nnm) time with a fast embedding for sketching. Via extensive experiments on fine-tuning vision models, we empirically validate the performance of RPVopt in both regression and classification settings, where it outperforms existing data selection methods across various settings, especially for small coresets.

1.1 Related Works

Due to the space limit, we focus on OED here and defer further discussions regarding the more general data selection problem to Appendix A.1.

Optimal experimental design. While standard OED focuses on the overdetermined scenario with $n \ge d$, efforts have been made to extend the notion of V-optimality to overparametrized setting, d > n [19, 20, 16]. Specifically, [19, 20] proposes design criteria for ridge regression in the general overparametrized setting. More recently, [16] considers overparametrized ridge regression with low intrinsic dimension in the context of finetuning and provides a selection criterion based on sketching that brings a sample complexity independent of d.

Fast algorithms for V-optimality. Despite the long history of OED, progress in provable algorithms for V-optimality [18, 17, 21] has taken place more recently and remains surprisingly sparse. In particular, [17, 21] introduced an optimization-based framework for a broad variety of optimality criteria, including the V-optimality, which provably finds a nearly optimal coreset in polynomial time. The framework consists of two stages: (i) solving a continuous relaxation of the original discrete optimization problem and (ii) rounding the continuous solution via regret minimization. However, solving the continuous relaxation can be prohibitively expensive despite its polynomial complexity [21]. Related to V-optimality, A(verage)-optimality is a more studied design criterion. Specifically, [22] shows that under mild conditioning assumptions, the classical Fedorov's exchange method [14] finds a nearly optimal coreset in polynomial time. Beyond computational tractability, [23] investigates and improves a set of fast algorithms for the A-optimal experimental design, including greedy removal [24], volume sampling [24], leverage score sampling [25], and dual set sparsification [26].

2 Data Selection under Low Intrinsic Dimension

Notations. Given any $n \in \mathbb{Z}_+$, let $[n] = \{1, \dots, n\}$. Let \mathbf{e}_n be the *n*-th canonical basis of the conformable dimension. For any set U, we denote |U| as the cardinality of U. Additionally, for any $n \in [|U|]$, let $\mathcal{C}(U,n) = \{S \subseteq U \mid |S| = n\}$. We adapt the standard asymptotic notations: for any functions $f, g : \mathbb{R}_+ \to \mathbb{R}_+$, we write f = O(g) or $f \lesssim g$ if there exists some constant C > 0 such that $f(x) \leq Cg(x)$ for all $x \in \mathbb{R}_+$; $f = \Omega(g)$ or $f \gtrsim g$ if g = O(f); $f \asymp g$ if f = O(g) and $f = \Omega(g)$. For any matrix \mathbf{A} , let $\sigma_1(\mathbf{A}) \geq \cdots \geq \sigma_{\operatorname{rank}(\mathbf{A})}(\mathbf{A}) \geq 0$ be the singular values; and denote \mathbf{A}^{\dagger} as the Moore-Penrose pseudoinverse. Additionally for any $k \leq \operatorname{rank}(\mathbf{A})$, let $\langle \mathbf{A} \rangle_k = \operatorname{argmin}_{\mathbf{B}: \operatorname{rank}(\mathbf{B}) \leq k} \|\mathbf{A} - \mathbf{B}\|_F$ be the optimal rank-k approximation of \mathbf{A} (characterized by the rank-k truncated SVD). For any symmetric matrices $\mathbf{A}, \mathbf{B} \in \mathbb{R}^{d \times d}$, we write $\mathbf{A} \succeq \mathbf{B}$ or $\mathbf{A} - \mathbf{B} \succeq 0$ if $\mathbf{A} - \mathbf{B}$ is positive semidefinite.

2.1 Low-dimensional Data Selection and V-optimal Design

Data distribution. Consider a data distribution P over $\mathcal{X} \times \mathbb{R}$ ($\mathcal{X} \subset \mathbb{R}^d$) characterized by the ground truth $\boldsymbol{\theta}_* \in \mathbb{R}^d$ and level of noise $\sigma > 0$: (i) $\mathbb{E}_{(\mathbf{x},y)\sim P}[y \mid \mathbf{x}] = \mathbf{x}^\top \boldsymbol{\theta}_*$, and (ii) $\mathbb{V}_{(\mathbf{x},y)\sim P}[y \mid \mathbf{x}] \leq \sigma^2$. Let $\mathbf{X} = [\mathbf{x}_1, \cdots, \mathbf{x}_N]^\top \in \mathbb{R}^{N \times d}$ be the data matrix associated with a huge set of N unlabeled samples $\{\mathbf{x}_i \in \mathbb{R}^d \mid i \in [N]\}$ drawn *i.i.d.* from P. For simplicity, we assume rank $(\mathbf{X}) = d$ and consider the fixed design setting with $\mathcal{X} = \mathbf{X}$ and a uniform marginal distribution $P(\mathbf{x}_i) = 1/N$ for all $i \in [N]$. Each \mathbf{x}_i is associated with an unknown label $y_i = \mathbf{x}_i^\top \boldsymbol{\theta}_* + z_i$ that can be queried with non-negligible cost, where z_i is an independent and zero-mean random variable with $\mathbb{V}[z_i] \leq \sigma^2$.

Learning problem. For any $S = \{i_1, \dots, i_n\} \in \mathcal{C}([N], n) = \{S \subset [N] \mid |S| = n\}$, let $\mathbf{X}_S = [\mathbf{x}_{i_1}, \dots, \mathbf{x}_{i_n}]^\top \in \mathbb{R}^{n \times d}$ be the data submatrix selected by S. Denote $\mathbf{\Sigma} = \frac{1}{N} \mathbf{X}^\top \mathbf{X}$ and $\mathbf{\Sigma}_S = \frac{1}{n} \mathbf{X}_S^\top \mathbf{X}_S$ as the $d \times d$ second moments. Given a target coreset size n < N, the goal of data selection is to find a nearly optimal data subset indexed by $S \in \mathcal{C}([N], n)$ such that by querying only n labels $\mathbf{y}_S \in \mathbb{R}^n$ associated with \mathbf{X}_S , one can learn a "good" approximation $\boldsymbol{\theta}_S$ of $\boldsymbol{\theta}_*$ from $(\mathbf{X}_S, \mathbf{y}_S)$. Consider a regression problem with ℓ_2 population loss, $L(\boldsymbol{\theta}) = \mathbb{E}_{(\mathbf{x},y) \sim P}[(\mathbf{x}^\top \boldsymbol{\theta} - y)^2]$. In the context of statistical learning, a "good" approximation of $\boldsymbol{\theta}_*$ generally refers to a $\boldsymbol{\theta} \in \mathbb{R}^d$ with low excess risk, $\text{ER}(\boldsymbol{\theta}) = L(\boldsymbol{\theta}) - L(\boldsymbol{\theta}_*) = \|\boldsymbol{\theta} - \boldsymbol{\theta}_*\|_{\mathbf{\Sigma}}^2$, where $\mathbf{\Sigma} \succ 0$ as $\text{rank}(\mathbf{X}) = d$.

Low- v.s. high-dimensional data selection. We refer to "low-dimensional" data selection as the case where the data dimension is lower than the coreset size, $d \le n$ (or more precisely, $d = \operatorname{rank}(\mathbf{X}_S)$), and therefore, θ_S is uniquely identified by an overdetermined system:

Low-dimensional:
$$d = \operatorname{rank}(\mathbf{X}_S), \quad \boldsymbol{\theta}_S = \operatorname*{argmin}_{\boldsymbol{\theta} \in \mathbb{R}^d} \frac{1}{n} \|\mathbf{X}_S \boldsymbol{\theta} - \mathbf{y}_S\|_2^2$$
 (1)

In contrast, "high-dimensional" data selection refer to an overparametrized problem with d > n (or more precisely, $d > \operatorname{rank}(\mathbf{X}_S)$), where $\boldsymbol{\theta}_S$ is learned through ridge regression with a suitable choice of regularization hyperparameter $\alpha > 0$:

High-dimensional :
$$d > \operatorname{rank}(\mathbf{X}_S), \quad \boldsymbol{\theta}_S = \operatorname*{argmin}_{\boldsymbol{\theta} \in \mathbb{R}^d} \frac{1}{n} \|\mathbf{X}_S \boldsymbol{\theta} - \mathbf{y}_S\|_2^2 + \alpha \|\boldsymbol{\theta}\|_2^2.$$
 (2)

V-optimal design. Classical OED studies the low-dimensional data selection problem where various optimality criteria [13] are introduced to characterize different notions of "distance" between θ_S and θ_* . For example, the A(verage)-optimality tr(Σ_S^{\dagger}) is associated with the Euclidean distance $\|\theta_S - \theta_*\|_2^2$; whereas the V(ariance)-optimality tr($\Sigma\Sigma_S^{\dagger}$) is arguably the most relevant criterion that directly controls the excess risk (*e.g.* see [15, Section 7.5.2] or [16, (1)]):

$$\mathbb{E}\left[\mathrm{ER}(\boldsymbol{\theta}_{S})\right] = \mathbb{E}\left[\left\|\boldsymbol{\theta}_{S} - \boldsymbol{\theta}_{*}\right\|_{\boldsymbol{\Sigma}}^{2}\right] \leq \frac{\sigma^{2}}{n} \operatorname{tr}(\boldsymbol{\Sigma}\boldsymbol{\Sigma}_{S}^{\dagger}).$$
(3)

2.2 High-dimensional Data Selection under Low Intrinsic Dimension

For data selection, a common and intriguing high-dimensional setting is learning problems with low intrinsic dimensions [7, 8] (*e.g.* finetuning). Specifically, [8] unveils the possibility of finetuning high-dimensional models with sample complexities proportional to their low intrinsic dimensions, which is impossible in general high-dimensional settings.

For high-dimensional data selection under low intrinsic dimension, [16] proposes to (i) find a lowdimensional subspace that encapsulates crucial information in data via sketching [27, 28, 29], and then (ii) select data by solving the OED problem in the resulting low-dimensional subspace. In this context, [16] introduces a data selection criterion that generalizes the notion of V-optimality:

Remark 2.1 ([16, Theorem 3.1]). Let $\overline{r} = \min\{t \in [r] \mid ||\langle \mathbf{X} \rangle_t||_F^2 \ge (1 - \frac{1}{N}) ||\mathbf{X}||_F^2\}$ be the intrinsic dimension of the dataset \mathbf{X} . Assume \mathbf{X} has a low intrinsic dimension: $\overline{r} \ll \min\{N, d\}$. Sketch \mathbf{X} via a Gaussian embedding $\mathbf{\Gamma} \in \mathbb{R}^{d \times m}$ with i.i.d. entries $\Gamma_{ij} \sim \mathcal{N}(0, 1/m)$ and embedding dimension $m \ge 11\overline{r}$ such that $\widetilde{\mathbf{\Sigma}} = \frac{1}{N} (\mathbf{X} \mathbf{\Gamma})^\top (\mathbf{X} \mathbf{\Gamma})$ and $\widetilde{\mathbf{\Sigma}}_S = \frac{1}{n} (\mathbf{X}_S \mathbf{\Gamma})^\top (\mathbf{X}_S \mathbf{\Gamma})$ for any $S \in \mathcal{C}([N], n)$. If $\sigma_{[1,1\overline{r}]}(\widetilde{\mathbf{\Sigma}}_S) \ge \gamma_S$ for some $\gamma_S > 0$, then with probability at least 0.9 over $\mathbf{\Gamma}$, there exists a regularization hyperparameter $\alpha > 0$ such that (2) satisfies

$$\mathbb{E}\left[\mathrm{ER}\left(\boldsymbol{\theta}_{S}\right)\right] \lesssim \underbrace{\frac{\sigma^{2}}{n} \operatorname{tr}(\widetilde{\boldsymbol{\Sigma}}(\widetilde{\boldsymbol{\Sigma}}_{S})^{\dagger})}_{variance} + \underbrace{\frac{\sigma^{2}}{n} \frac{1}{m\gamma_{S}} \|\widetilde{\boldsymbol{\Sigma}}(\widetilde{\boldsymbol{\Sigma}}_{S})^{\dagger}\|_{2} \operatorname{tr}(\boldsymbol{\Sigma})}_{sketching \ error} + \underbrace{\frac{1}{n} \|\widetilde{\boldsymbol{\Sigma}}(\widetilde{\boldsymbol{\Sigma}}_{S})^{\dagger}\|_{2} \operatorname{tr}(\boldsymbol{\Sigma}) \|\boldsymbol{\theta}_{*}\|_{2}^{2}}_{bias}.$$
 (4)

In particular, when $\|\widetilde{\Sigma}(\widetilde{\Sigma}_S)^{\dagger}\|_2 \leq c_S$, under mild regularity assumptions $\sigma^2 = O(1), \|\boldsymbol{\theta}_*\|_2^2 = O(1),$ and $\operatorname{tr}(\boldsymbol{\Sigma}) = O(\bar{r})$, taking $m = \max\{\sqrt{\operatorname{tr}(\boldsymbol{\Sigma})/\gamma_S}, 11\bar{r}\}$ leads to $\mathbb{E}[\operatorname{ER}(\boldsymbol{\theta}_S)] \lesssim c_S \bar{r}/n$, *i.e.* a sample complexity proportional to the low intrinsic dimension \overline{r} .

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Observing that the generalization of data selection in (4) is governed by $\operatorname{tr}(\hat{\Sigma}(\hat{\Sigma}_S)^{\dagger}) \geq \|\hat{\Sigma}(\hat{\Sigma}_S)^{\dagger}\|_2$, in this section, we introduce a fast and effective data selection algorithm based on sketching and random pivoting that adaptively samples data to optimize $\operatorname{tr}(\widehat{\Sigma}(\widehat{\Sigma}_S)^{\dagger})$ locally.

Dimension reduction via sketching. Algorithm 3.1 starts by embedding the high-dimensional data to a random low-dimensional subspace via sketching: $\widetilde{\mathbf{X}} = \mathbf{X} \mathbf{\Gamma} \in \mathbb{R}^{N \times m}$, where a common choice of Γ is a Gaussian random matrix (vide [27, 28] for a comprehensive overview of sketching).

Randomly pivoted QR. With $\widetilde{\mathbf{X}}$, Algorithm 3.1 selects the first *m* samples via randomly pivoted QR [30]: Initializing $\widetilde{\mathbf{X}}^{(0)} = [\widetilde{\mathbf{x}}_1^{(0)}, \cdots, \widetilde{\mathbf{x}}_N^{(0)}]^\top = \widetilde{\mathbf{X}} \in \mathbb{R}^{N \times m}$ and $S_0 = \emptyset$, for $t \in [m]$:

(i) Sample i_t from $[N] \setminus S_{t-1}$ with probability $p_i = \|\widetilde{\mathbf{x}}_i^{(t-1)}\|_2^2 / \|\widetilde{\mathbf{X}}^{(t-1)}\|_F^2$ for all $i \in [N] \setminus S_{t-1}$; $\widetilde{\sim}$ (i) $\widetilde{\sim}$ (i = 1) $\widetilde{\sim}$ (i = 1) $\widetilde{\sim}$ (t = 1) $\widetilde{\sim}$ (t = 1). \top $\widetilde{\sim}$ (t = 1). (1

ii) Update
$$S_t = S_{t-1} \cup \{i_t\}$$
 and $\mathbf{X}^{(t)} = \mathbf{X}^{(t-1)} - \mathbf{X}^{(t-1)} \widetilde{\mathbf{x}}_{i_t}^{(t-1)} (\widetilde{\mathbf{x}}_{i_t}^{(t-1)})^\top / \|\widetilde{\mathbf{x}}_{i_t}^{(t-1)}\|_2^{2.2}$

When rank(\mathbf{X}) = d, sketching via a Gaussian embedding with $m \leq d$ provides rank($\widetilde{\mathbf{X}}$) = m with probability one. Then, the Gram-Schmidt process ensures that randomly pivoted QR selects m linearly independent samples, *i.e.* rank $(\mathbf{X}_{S_m}) = m$. It is worth noticing that random pivoted QR is effectively replacing the greedy pivoting in the classical row pivoted QR [32] with adaptive square norm sampling, which achieves better accuracy and robustness in both theory and practice [30].

Adaptive V-optimal design via random pivoting. With the first *m* linearly independent samples, Algorithm 3.1 continues by adaptively sampling the remaining n - m data according to the Voptimality over $\widetilde{\mathbf{X}}$. In particular, since $\operatorname{rank}(\widetilde{\mathbf{X}}_{S_m}) = m$, for any subsequent $S \supset S_m$, $\operatorname{rank}(\widetilde{\mathbf{X}}_S) = m$. m. Then, the Woodbury matrix identity [33] implies that for any $S \supset \hat{S}_m$ and $i \in [N] \setminus S$,

$$(\widetilde{\mathbf{X}}_{S}^{\top}\widetilde{\mathbf{X}}_{S} + \widetilde{\mathbf{x}}_{i}\widetilde{\mathbf{x}}_{i}^{\top})^{-1} = (\widetilde{\mathbf{X}}_{S}^{\top}\widetilde{\mathbf{X}}_{S})^{-1} - \frac{(\widetilde{\mathbf{X}}_{S}^{\top}\widetilde{\mathbf{X}}_{S})^{-1}\widetilde{\mathbf{x}}_{i}\widetilde{\mathbf{x}}_{i}^{\top}(\widetilde{\mathbf{X}}_{S}^{\top}\widetilde{\mathbf{X}}_{S})^{-1}}{1 + \widetilde{\mathbf{x}}_{i}^{\top}(\widetilde{\mathbf{X}}_{S}^{\top}\widetilde{\mathbf{X}}_{S})^{-1}\widetilde{\mathbf{x}}_{i}},$$
(5)

and therefore, $\operatorname{tr}(\widetilde{\mathbf{X}}^{\top}\widetilde{\mathbf{X}}(\widetilde{\mathbf{X}}_{S\cup\{i\}}^{\top}\widetilde{\mathbf{X}}_{S\cup\{i\}})^{-1}) = \operatorname{tr}(\widetilde{\mathbf{X}}^{\top}\widetilde{\mathbf{X}}(\widetilde{\mathbf{X}}_{S}^{\top}\widetilde{\mathbf{X}}_{S})^{-1}) - \Delta_{S}(\widetilde{\mathbf{x}}_{i})$ where $\Delta_{S}(\widetilde{\mathbf{x}}_{i}) = \sum_{i=1}^{N} \sum_{j=1}^{N} \sum_{i=1}^{N} \sum_{j=1}^{N} \sum_{j=1}^{N} \sum_{i=1}^{N} \sum_{j=1}^{N} \sum_{j=1}^{N} \sum_{i=1}^{N} \sum_{j=1}^{N} \sum_{i=1}^{N} \sum_{j=1}^{N} \sum_{j=1}^{N} \sum_{i=1}^{N} \sum_{j=1}^{N} \sum_{j=1}^{N} \sum_{i=1}^{N} \sum_{j=1}^{N} \sum_{j=1}^{N} \sum_{i=1}^{N} \sum_{j=1}^{N} \sum_{i=1}^{N} \sum_{j=1}^{N} \sum_{j=1}^{N} \sum_{i=1}^{N} \sum_{j=1}^{N} \sum_{j=1}^{N} \sum_{i=1}^{N} \sum_{j=1}^{N} \sum_{i=1}^{N} \sum_{j=1}^{N} \sum_{j=1}^{N} \sum_{i=1}^{N} \sum_{i=1}^{N} \sum_{i=1}^{N} \sum_{i=1}^{N} \sum_{i=1}^{N} \sum_{j=1}^{N} \sum_{i=1}^{N} \sum_{j=1}^{N} \sum_{i=1}^{N} \sum_{$ $\|\widetilde{\mathbf{X}}(\widetilde{\mathbf{X}}_{S}^{\top}\widetilde{\mathbf{X}}_{S})^{-1}\widetilde{\mathbf{x}}_{i}\|_{2}^{2}/(1+\widetilde{\mathbf{x}}_{i}^{\top}(\widetilde{\mathbf{X}}_{S}^{\top}\widetilde{\mathbf{X}}_{S})^{-1}\widetilde{\mathbf{x}}_{i}).$ Since $\operatorname{tr}(\widetilde{\mathbf{\Sigma}}\widetilde{\mathbf{\Sigma}}_{S_{n}}^{-1}) = \frac{n}{N}\operatorname{tr}(\widetilde{\mathbf{X}}^{\top}\widetilde{\mathbf{X}}(\widetilde{\mathbf{X}}_{S_{n}}^{\top}\widetilde{\mathbf{X}}_{S_{n}})^{-1}),$ for given $S \supset S_{m}$, picking $i \in [N] \setminus S$ with the maximum $\Delta_{S}(\widetilde{\mathbf{x}}_{i})$ brings the optimal reduction in $\operatorname{tr}(\widetilde{\Sigma}\widetilde{\Sigma}_{S_{n}}^{-1})$ locally, leading to a natural greedy algorithm.

To alleviate the potential suboptimality caused by the local optimality, instead of greedy selection, we inject randomness by sampling proportional to $\exp(\Delta_{S_{t-1}}(\tilde{\mathbf{x}}_i)/\tau)$, with the randomness controlled by a temperature hyperparameter τ .

Notice that the overall asymptotic complexity of Algorithm 3.1 is O(Ndm+Nnm) with the Gaussian embedding, whereas leveraging more efficient sparse embeddings [34, 35, 36] can further bring down the complexity to $O(nnz(\mathbf{X}) + Nnm)$ in practice [37], where $nnz(\mathbf{X}) \leq Nd$ denotes the number of nonzero entries in X. This matches the complexity of ridge leverage score sampling with fast leverage score approximation [38, 39, 40], which (to the best of our knowledge) is one of the most efficient provable algorithms for A-optimality [23] and data selection [39]. In Section 4.1, we empirically demonstrate that RPVopt outperforms ridge leverage score sampling in data selection for regression, especially when the coreset size is small. The theoretical guarantee for RPVopt that matches its empirical performance remains an exciting open problem.

4 **Experiments**

In this section, we evaluate the performance of RPVopt in Algorithm 3.1 on different settings. We first show the effectiveness of our proposed method on regression tasks then extend the experimental

²This Gram-Schmidt process is numerically unstable with floating point arithmetic. In practice, a stable implementation like [31, Algorithm 3.1] is used.

Algorithm 3.1 Randomly Pivoted V-optimal Design (RPVopt)

Input: $\mathbf{X} \in \mathbb{R}^{N \times d}$, coreset size *n*, temperature $\tau > 0$, embedding dimension m < n. 1: (Draw a Gaussian embedding $\mathbf{\Gamma} \in \mathbb{R}^{d \times m}$ with *i.i.d.* entries $\mathbf{\Gamma}_{ij} \sim (0, 1/m)$.) 2: (Compute the sketching $\widetilde{\mathbf{X}} = \mathbf{X} \mathbf{\Gamma} = [\widetilde{\mathbf{x}}_1, \cdots, \widetilde{\mathbf{x}}_N]^\top \in \mathbb{R}^{N \times m}$.) $\triangleright O(Ndm)$ 3: Select $S_m \in \mathcal{C}([N], m)$ from $\widetilde{\mathbf{X}}$ via randomly pivoted QR. $\triangleright O(Nm^2)$ 4: $\mathbf{Y}_{(m)} \leftarrow \widetilde{\mathbf{X}}(\widetilde{\mathbf{X}}_{S_m}^{\top} \widetilde{\mathbf{X}}_{S_m})^{-1} \in \mathbb{R}^{N \times m}$. 5: for $t = m + 1, \cdots, n$ do $\triangleright O(Nm^2 + m^3)$ $\Delta_{S_{t-1}}(\widetilde{\mathbf{x}}_i) \leftarrow \|\mathbf{Y}_{(t-1)}\widetilde{\mathbf{x}}_i\|_2^2 / (1 + \mathbf{e}_i^\top \mathbf{Y}_{(t-1)}\widetilde{\mathbf{x}}_i) \,\forall \, i \in \overline{S_{t-1}}.$ $\triangleright O(Nm)$ 6: $\mathbf{p} = (p_1, \cdots, p_N) \leftarrow \mathbf{0}_{[N]}, p_i \leftarrow \exp(\Delta_{S_{t-1}}(\widetilde{\mathbf{x}}_i)/\tau) \; \forall \; i \in \overline{S_{t-1}}.$ 7: Sample $i_t \sim \mathbf{p} / \|\mathbf{p}\|_1$ 8: $S_t \leftarrow S_{t-1} \cup \{i_t\}.$ 9: $\mathbf{Y}_{(t)} \leftarrow \mathbf{Y}_{(t-1)} - (\mathbf{Y}_{(t-1)} \widetilde{\mathbf{x}}_{i_t}) (\mathbf{e}_{i_t}^\top \mathbf{Y}_{(t-1)}) / (1 + \mathbf{e}_{i_t}^\top \mathbf{Y}_{(t-1)} \widetilde{\mathbf{x}}_{i_t}).$ 10: $\triangleright O(Nm)$ return $S_n \in \mathcal{C}([N], n)$.

protocol to include classification tasks. Due to the limit constraint, the detailed configurations are provided in Appendix B.

4.1 Regression

Datasets and network architectures. We conduct regression experiments on UTKFace [41], which is a dataset for age estimation, with CLIP [1] and ResNet18 [42] backbones. While we examine linear probing on CLIP (ViT-B/32), we fine-tune the projections layer and the classifier of ResNet18 to represent the low- and high-dimensional settings, respectively. For both experiments, we utilize the Adam optimizer [43] with a batch size of 128 and an initial learning rate of 0.1.

Baselines. We evaluate our method by comparing it against notable unsupervised data selection methods for regression: (1) **Uniform Sampling** randomly all samples with equal probability, (2) **Adaptive Sampling** [44, 30] progressively sampling data based on their squared norms and adaptively eliminating the spanning subspace of the selected samples, (3) **Ridge Leverage Score Sampling** [38, 39, 40] extending classical leverage score sampling [45] to high dimensions, measuring of the influence that individual data points have on linear regression models, (4) **Greedy** [46] choosing a subset such that the bound between an average loss over any given subset of the dataset and the remaining data points is minimized, (5) **Herding** [47] greedily selects samples to minimize the selection set center and full dataset center in the feature space.

Table 1: Mean Absolute Error (the lower the better) on UTKFace with a linear regressor trained on top of frozen features from a pre-trained CLIP (ViT-B/32). We use the **bold** font to indicate the best method for each coreset size.

| Method | 100 | 200 | 500 | 1000 | 2000 | 3000 |
|------------------|------------------|-----------------|---------------------|-----------------|-----------------|-----------------|
| Uniform Sampling | 10.55 ± 3.09 | 8.94 ± 3.48 | 6.09 ± 0.42 | 4.70 ± 0.23 | 3.92 ± 0.16 | 3.68 ± 0.15 |
| Adaptive | 6.02 ± 0.53 | 4.75 ± 0.14 | 4.40 ± 0.14 | N/A | N/A | N/A |
| Greedy | 10.40 ± 1.21 | 7.56 ± 0.18 | 6.43 ± 0.09 | 5.51 ± 0.19 | 4.87 ± 0.03 | 4.37 ± 0.08 |
| Herding | 17.57 ± 0.01 | 13.41 ± 0.01 | 8.47 ± 0.01 | 5.79 ± 0.01 | 4.19 ± 0.01 | 3.53 ± 0.01 |
| R-leverage | 5.44 ± 0.01 | 4.79 ± 0.02 | 4.36 ± 0.01 | 3.86 ± 0.01 | 3.61 ± 0.01 | 3.53 ± 0.04 |
| RPVopt | 5.14 ± 0.30 | 4.43 ± 0.12 | $\bf 4.13 \pm 0.24$ | 3.82 ± 0.07 | 3.67 ± 0.05 | 3.47 ± 0.14 |

The results for linear probing are provided in Table 1, where our method remarkably outperforms comparative baselines on UTKFace, especially for smaller coreset sizes n. For n = 100, 200, 500, RPVopt exceeds the performance of the second-best method, R-leverage, by approximately 0.3 MAE, and achieves a Mean Absolute Error reduction of 30 - 50% compared to Uniform Sampling.

Table 2: Mean Absolute Error on UTK in fine-tuning the last two layers of ResNet18.

| | | | | 0 | 2 | | |
|------------------|------------------|------------------|-----------------|------------------|-----------------|-----------------|--|
| Method | 100 | 200 | 500 | 1000 | 2000 | 3000 | |
| Uniform Sampling | 8.43 ± 1.54 | 8.13 ± 0.52 | 6.62 ± 0.38 | 5.44 ± 0.53 | 5.02 ± 0.67 | 4.40 ± 0.49 | |
| Adaptive | 9.60 ± 0.10 | 8.29 ± 0.91 | 6.28 ± 0.77 | N/A | N/A | N/A | |
| Greedy | 10.82 ± 1.29 | 9.83 ± 0.51 | 6.98 ± 0.71 | 5.95 ± 0.22 | 5.33 ± 0.74 | 4.60 ± 0.19 | |
| Herding | 23.08 ± 2.11 | 22.33 ± 1.49 | 19.68 ± 0.02 | 20.24 ± 0.13 | 6.31 ± 1.49 | 5.39 ± 0.58 | |
| R-leverage | 12.20 ± 0.19 | 10.68 ± 0.37 | 7.71 ± 0.33 | 5.50 ± 0.44 | 5.25 ± 0.42 | 4.20 ± 0.44 | |
| RPVopt | 8.39 ± 0.19 | 7.33 ± 0.61 | 5.74 ± 0.31 | 4.74 ± 0.16 | 4.58 ± 0.33 | 4.32 ± 0.27 | |
| | | | | | | | |

In Table 2, we finetune the last two layers of ResNet18 [42] using the same optimization setting with the above linear probing experiment. Similarly, RPVopt consistently achieves the best performance

among all baselines. It is worth noting that while some selected comparative underperform relative to the uniform sampling baseline, particularly at higher pruning rates, our method consistently surpasses this baseline across various coreset sizes. For the UTKFace experiments, the computational cost associated with the Adaptive method is prohibitively expensive, rendering it impractical for large core sizes, i.e., greater than 500.

4.2 Classification

To evaluate the performance of our methods beyond the regression task, we conduct experiments on the CIFAR10 [48] and StanfordCars [49] datasets in the classification setting. Apart from those baselines described in the above experiments, we compare our methods with the following methods based on the DeepCore benchmark [50]. **Contextual Diversity** [51] proposes using contextual diversity to select diverse samples. **Glister** [52] uses bi-level optimization to optimize the selection set. **GraNd** [53] uses the gradient norm of warmup trained model to select samples. **Forgetting** [54] uses the forgetting events (correctly classified samples that are later misclassified during the training process) as the selection criterion. **DeepFool** [55] uses the adversarial attacking strength to identify the samples that are close to the decision boundary and select them. **Uncertainty-Based Methods** [56] use the model's uncertainty metric (entropy, margin, confidence) to construct the selection set.

| Method | Metric | 500 | 1000 | 1500 | 2000 | 2500 | 3000 | 3500 | 4000 |
|---------------------------|--------|------------------|------------------|------------------|------------------|------------------|------------------|---|------------------|
| Uniform Compliant | Acc | 38.90 ± 0.46 | 54.60 ± 0.46 | 62.60 ± 0.23 | 67.63 ± 0.17 | 70.59 ± 0.19 | 72.49 ± 0.19 | 74.16 ± 0.22 | 75.40 ± 0.16 |
| Uniform Sampling | F1 | 32.30 ± 0.43 | 49.94 ± 0.56 | 58.99 ± 0.23 | 64.54 ± 0.18 | 67.79 ± 0.23 | 70.00 ± 0.20 | 71.77 ± 0.23 | 73.14 ± 0.12 |
| Handing [47] | Acc | 38.86 ± 0.40 | 54.95 ± 0.33 | 63.44 ± 0.31 | 67.22 ± 0.16 | 71.02 ± 0.13 | 73.17 ± 0.22 | 74.64 ± 0.18 | 75.71 ± 0.29 |
| Herding [47] | F1 | 31.80 ± 0.32 | 50.14 ± 0.51 | 59.75 ± 0.32 | 64.07 ± 0.23 | 68.28 ± 0.15 | 70.64 ± 0.28 | 72.22 ± 0.26 | 73.26 ± 0.39 |
| Contextual Diversity [51] | Acc | 38.05 ± 0.39 | 53.87 ± 0.38 | 62.36 ± 0.18 | 67.64 ± 0.13 | 70.82 ± 0.23 | 72.66 ± 0.12 | 74.46 ± 0.17 | 75.77 ± 0.12 |
| Contextual Diversity [51] | F1 | 31.25 ± 0.50 | 48.99 ± 0.29 | 58.77 ± 0.24 | 64.51 ± 0.17 | 68.18 ± 0.25 | 70.05 ± 0.11 | 72.13 ± 0.15 | 73.35 ± 0.07 |
| Clister [52] | Acc | 39.15 ± 0.23 | 54.57 ± 0.39 | 62.67 ± 0.19 | 67.60 ± 0.24 | 70.85 ± 0.27 | 73.07 ± 0.26 | 74.63 ± 0.21 | 76.00 ± 0.20 |
| Glister [52] | F1 | 32.32 ± 0.31 | 49.72 ± 0.53 | 58.80 ± 0.32 | 64.50 ± 0.34 | 68.07 ± 0.38 | 70.47 ± 0.35 | 72.18 ± 0.25 | 73.69 ± 0.24 |
| | Acc | 38.52 ± 0.06 | 54.65 ± 0.12 | 62.96 ± 0.10 | 67.27 ± 0.07 | 70.38 ± 0.07 | 72.56 ± 0.05 | 74.67 ± 0.06 | 75.77 ± 0.12 |
| Grand [55] | F1 | 32.34 ± 0.10 | 49.89 ± 0.14 | 59.09 ± 0.13 | 64.04 ± 0.09 | 67.48 ± 0.09 | 69.81 ± 0.08 | 72.13 ± 0.05 | 73.44 ± 0.13 |
| Equation [54] | Acc | 38.18 ± 0.43 | 54.84 ± 0.23 | 62.55 ± 0.15 | 67.59 ± 0.10 | 70.99 ± 0.05 | 72.54 ± 0.07 | 74.81 ± 0.05 | 75.74 ± 0.01 |
| Forgetting [54] | F1 | 31.67 ± 0.39 | 50.02 ± 0.20 | 58.64 ± 0.16 | 64.85 ± 0.13 | 68.53 ± 0.07 | 70.30 ± 0.05 | $\begin{array}{ccc} .07 & 74.81 \pm 0.05 \\ .05 & 72.59 \pm 0.04 \end{array}$ | 73.74 ± 0.02 |
| DeepEool [55] | Acc | 38.69 ± 0.64 | 54.85 ± 0.33 | 62.90 ± 0.21 | 67.77 ± 0.29 | 70.73 ± 0.22 | 73.24 ± 0.22 | 74.57 ± 0.23 | 75.71 ± 0.15 |
| Deepi ooi [55] | F1 | 31.67 ± 0.68 | 49.79 ± 0.53 | 58.93 ± 0.32 | 64.42 ± 0.27 | 67.91 ± 0.15 | 70.73 ± 0.20 | $\begin{array}{cccccccccccccccccccccccccccccccccccc$ | 73.39 ± 0.20 |
| Entropy [56] | Acc | 39.68 ± 0.37 | 54.78 ± 0.22 | 63.42 ± 0.18 | 67.95 ± 0.11 | 71.00 ± 0.10 | 73.28 ± 0.10 | 75.02 ± 0.08 | 75.82 ± 0.06 |
| Entropy [50] | F1 | 32.53 ± 0.53 | 49.57 ± 0.29 | 59.62 ± 0.25 | 64.55 ± 0.10 | 67.95 ± 0.12 | 70.68 ± 0.12 | 72.46 ± 0.12 | 73.29 ± 0.04 |
| Morgin [56] | Acc | 39.33 ± 0.22 | 54.36 ± 0.17 | 62.66 ± 0.12 | 67.53 ± 0.14 | 71.19 ± 0.09 | 73.09 ± 0.14 | 74.66 ± 0.11 | 75.57 ± 0.13 |
| Margin [50] | F1 | 32.03 ± 0.30 | 49.00 ± 0.23 | 58.62 ± 0.21 | 64.16 ± 0.15 | 68.33 ± 0.14 | 70.37 ± 0.17 | 72.03 ± 0.11 | 73.14 ± 0.20 |
| Least Confidence [56] | Acc | 39.00 ± 0.25 | 54.14 ± 0.30 | 63.23 ± 0.20 | 67.68 ± 0.11 | 70.99 ± 0.14 | 73.04 ± 0.05 | 74.65 ± 0.09 | 75.58 ± 0.08 |
| Least Connuelice [50] | F1 | 31.83 ± 0.21 | 48.90 ± 0.37 | 59.31 ± 0.29 | 64.09 ± 0.20 | 68.03 ± 0.20 | 70.30 ± 0.07 | 72.02 ± 0.10 | 73.15 ± 0.12 |
| DDVont | Acc | 40.39 ± 0.35 | 55.48 ± 0.40 | 63.47 ± 0.30 | 68.45 ± 0.15 | 72.13 ± 0.23 | 73.72 ± 0.15 | 75.76 ± 0.24 | 76.31 ± 0.20 |
| Kr vopi | F1 | 33.40 ± 0.25 | 50.35 ± 0.57 | 59.88 ± 0.39 | 65.35 ± 0.17 | 69.29 ± 0.31 | 71.45 ± 0.20 | 73.50 ± 0.28 | 73.99 ± 0.24 |

Table 3: Linear Probing performance of CLIP on StanfordCars with different data pruning methods.

We use the linear probing and two-layer finetuning as the learning problem to evaluate the performance of our method on the CIFAR10 [48] as the standard homogenous dataset and the StanfordCars [49] as the challenging non-homogeneous dataset. While the results of CIFAR10 are deferred to the appendix, Table 3 shows the results of linear probing on StanfordCars on different coreset sizes, ranging from 500 to 4000. As can be seen, our method always achieves the best test accuracy and F1 scores in all settings. Notably, for the coreset size of 500, RPVopt exceeds the second-best method by 1.4% accuracy.

| Table 4: | Baselines p | erforman | ce on Star | nfordCars | when fine | -tuning th | ne last two | layers of | ResNet18. |
|----------|-------------|----------|------------|-----------|-----------|------------|-------------|-----------|-----------|
| Method | Met | ric 500 | 1000 | 1500 | 2000 | 2500 | 3000 | 3500 | 4000 |

| Method | Metric | 500 | 1000 | 1500 | 2000 | 2500 | 3000 | 3500 | 4000 |
|---------------------------|--------|-----------------------------------|------------------------------------|------------------------------------|------------------------------------|------------------------------------|------------------------------------|---|------------------------------------|
| Uniform Sampling | Acc | 10.69 ± 0.17 | 18.29 ± 0.34 | 24.74 ± 0.36 | 29.19 ± 0.37 | 32.77 ± 0.31 | 35.69 ± 0.35 | 38.02 ± 0.31 | 40.35 ± 0.26 |
| Uniform Sampling | F1 | 7.70 ± 0.21 | 15.29 ± 0.28 | 21.72 ± 0.34 | 26.14 ± 0.39 | 29.83 ± 0.30 | 32.80 ± 0.37 | 35.16 ± 0.30 | 37.51 ± 0.23 |
| Herding [47] | Acc | 11.11 ± 0.31 | 18.49 ± 0.45 | 24.53 ± 0.23 | $\textbf{29.19} \pm \textbf{0.21}$ | 32.42 ± 0.16 | 35.83 ± 0.24 | 38.30 ± 0.19 | 40.51 ± 0.19 |
| Herding [47] | F1 | 8.06 ± 0.25 | 15.46 ± 0.36 | 21.57 ± 0.30 | 25.90 ± 0.24 | 29.48 ± 0.23 | 32.89 ± 0.27 | $\begin{array}{c c c c c c c c c c c c c c c c c c c $ | 37.56 ± 0.21 |
| Contactual Diversity [51] | Acc | 10.30 ± 0.19 | 18.12 ± 0.22 | 24.47 ± 0.33 | 28.50 ± 0.34 | 32.66 ± 0.27 | 35.67 ± 0.32 | 38.31 ± 0.15 | 40.53 ± 0.18 |
| Contextual Diversity [51] | F1 | 7.66 ± 0.25 | 15.29 ± 0.23 | 21.81 ± 0.26 | 25.65 ± 0.40 | 29.79 ± 0.29 | 32.86 ± 0.31 | 35.55 ± 0.14 | 37.81 ± 0.23 |
| GraNd [52] | Acc | 10.72 ± 0.08 | 18.51 ± 0.21 | 24.33 ± 0.29 | 28.59 ± 0.17 | 32.67 ± 0.20 | 35.83 ± 0.16 | $\textbf{38.58} \pm \textbf{0.15}$ | $\textbf{40.70} \pm \textbf{0.11}$ |
| Glaind [55] | F1 | 7.82 ± 0.08 | 15.51 ± 0.20 | 21.18 ± 0.28 | 25.66 ± 0.15 | 29.70 ± 0.22 | 32.76 ± 0.16 | $\textbf{35.72} \pm \textbf{0.15}$ | 37.83 ± 0.11 |
| Forgetting [54] | Acc | 10.46 ± 0.26 | 18.80 ± 0.28 | 24.16 ± 0.21 | 28.61 ± 0.31 | 32.48 ± 0.28 | 35.18 ± 0.24 | 37.78 ± 0.22 | 40.24 ± 0.13 |
| Torgetting [54] | F1 | 7.46 ± 0.14 | 15.52 ± 0.20 | 21.06 ± 0.23 | 25.64 ± 0.25 | 29.58 ± 0.30 | 32.38 ± 0.20 | 35.16 ± 0.18 | 37.41 ± 0.14 |
| DeepFool [55] | Acc | 10.65 ± 0.29 | 18.52 ± 0.18 | $\textbf{24.97} \pm \textbf{0.20}$ | 29.02 ± 0.17 | 32.60 ± 0.18 | 35.59 ± 0.24 | 38.20 ± 0.22 | 39.98 ± 0.35 |
| Deepi 001 [55] | F1 | 7.89 ± 0.18 | 15.44 ± 0.23 | $\textbf{22.11} \pm \textbf{0.11}$ | 26.08 ± 0.29 | 29.83 ± 0.27 | 32.92 ± 0.33 | 35.47 ± 0.22 | 37.28 ± 0.40 |
| Entropy [56] | Acc | 10.30 ± 0.07 | 18.48 ± 0.13 | 24.25 ± 0.26 | 28.87 ± 0.13 | 32.84 ± 0.20 | 35.64 ± 0.20 | 37.96 ± 0.11 | 40.29 ± 0.27 |
| Endopy [50] | F1 | 7.69 ± 0.11 | 15.31 ± 0.23 | 21.24 ± 0.24 | 25.95 ± 0.17 | 30.03 ± 0.17 | 32.85 ± 0.23 | $\begin{array}{c} 35.16 \pm 0.30\\ 38.30 \pm 0.19\\ 35.50 \pm 0.22\\ 38.31 \pm 0.15\\ 35.55 \pm 0.14\\ 38.58 \pm 0.15\\ 35.75 \pm 0.14\\ 38.72 \pm 0.15\\ 37.78 \pm 0.22\\ 35.16 \pm 0.18\\ 38.20 \pm 0.22\\ 35.47 \pm 0.22\\ 37.96 \pm 0.11\\ 38.27 \pm 0.20\\ 35.61 \pm 0.12\\ 38.27 \pm 0.20\\ 35.61 \pm 0.17\\ 38.25 \pm 0.20\\ 35.42 \pm 0.16\\ 38.57 \pm 0.12\\ 35.68 \pm 0.15\\ 35.68 \pm 0$ | 37.33 ± 0.34 |
| Margin [56] | Acc | 10.58 ± 0.32 | 18.37 ± 0.26 | 24.36 ± 0.19 | 29.18 ± 0.12 | 32.73 ± 0.15 | 35.67 ± 0.30 | 38.27 ± 0.20 | 40.58 ± 0.06 |
| Margin [50] | F1 | 7.93 ± 0.22 | 15.41 ± 0.19 | 21.33 ± 0.22 | 26.15 ± 0.12 | 29.66 ± 0.05 | 32.86 ± 0.30 | 35.61 ± 0.17 | 37.77 ± 0.07 |
| LeastConfidence [56] | Acc | 10.64 ± 0.23 | 18.45 ± 0.30 | 24.72 ± 0.20 | 29.05 ± 0.07 | $\textbf{32.88} \pm \textbf{0.13}$ | 35.66 ± 0.18 | 38.25 ± 0.20 | 39.91 ± 0.09 |
| Eeasteonnuenee [50] | F1 | 7.80 ± 0.10 | 15.47 ± 0.37 | 21.75 ± 0.25 | 26.18 ± 0.04 | 30.03 ± 0.14 | 32.79 ± 0.15 | 35.42 ± 0.16 | 37.14 ± 0.12 |
| DDVant | Acc | 11.12 ± 0.21 | $\textbf{19.11} \pm \textbf{0.24}$ | 24.82 ± 0.15 | 29.13 ± 0.27 | 32.70 ± 0.19 | $\textbf{36.05} \pm \textbf{0.27}$ | 38.57 ± 0.12 | 40.56 ± 0.24 |
| кгуорі | F1 | $\textbf{8.18} \pm \textbf{0.16}$ | $\textbf{16.19} \pm \textbf{0.23}$ | 22.09 ± 0.21 | $\textbf{26.43} \pm \textbf{0.31}$ | $\textbf{30.33} \pm \textbf{0.23}$ | $\textbf{33.32} \pm \textbf{0.27}$ | 35.68 ± 0.15 | $\textbf{37.87} \pm \textbf{0.22}$ |

We also evaluate the performance of comparative methods finetuning the last two-layer of ResNet18 [42]. In Table 4, we showcase the results on StanfordCars, where RPVopt demonstrates impressive efficiency, boosting the performance of uniform sampling across different setups.

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A Additional Discussions

A.1 Additional Related Works

Data selection. Recent data selection methods identify important samples through training dynamics [54, 53], yielding additional annotation and computational costs, unaligned with the original goal of selecting data to reduce training costs. Label-free alternatives evaluate the importance of data via geometric properties in the embedding space [57, 51, 58]. These methods remove redundancy to form diverse, representative coresets without extensive labeling or (early-stage) training. This underlying idea of data selection based on geometric information is closely related to various widely studied problems like coreset selection [59, 28, 39, 60], active learning [61, 62, 63], and matrix skeletonization [64, 65, 66, 30, 31, 67]. More recent work named Variance Alignment Score (VAS) [68] and Sketchy Moment Matching [16] aligns some high-level statistics of the selected samples with that of the original data distribution, and additionally enhances model performance through data filtering or gradient sketching ideas respectively. These advances highlight the value of selecting informative and diverse coreset, especially in complex tasks.

A.2 Limitations and Future Directions

In this work, we introduce a fast data selection algorithm, RPVopt, for high-dimensional learning problems with low intrinsic dimensions. Concretely, RPVopt leverages the data selection criterion proposed in [16], first exploring the low intrinsic dimension in data via sketching, and then exploiting the information in the resulting low-dimensional subspace by adaptively sampling data that optimize the selection criterion locally. The appealing empirical performance of RPVopt is demonstrated in both regression and classification settings. A natural question regarding the theoretical guarantee for RPVopt remains open and is a work in progress.

Beyond the theoretical guarantee, the potentials and limitations of RPVopt are not fully understood in the current stage. First, while RPVopt is inspired by the analysis for regression problems, its competitive performance extends to the classification setting in practice. Second, the strong performance of RPVopt for unsupervised data selection on imbalanced classification tasks (*e.g.*, StanfordCars) suggests its potential in the context of distributionally robust data selection [69], beyond the classical statistical learning setting under the *i.i.d.* sampling assumption. Understanding the mechanism behind RPVopt in more comprehensive settings like classification and distributionally robust learning is an exciting future direction.

B Experiment Details and Additional Results

Due to the space constraint, some details were omitted in the main paper. We here provide the detailed training configuration in Section B.1 and additional experiment results in Section B.2.

B.1 Hyperparameter Selection and Training Details

We sweep the sketching dimension $m \in \{32, 64, 128, 256, 512\}$, the block size $b \in \{5, 10, 15, 20\}$ and temperature $\tau = e^{-3}$ for all experiments. We use the feature before the last linear layer in linear probing and the last-two layer gradients in two-layer finetuning to perform sketching and selection. For linear probing, we train the model 50 epochs with Adam optimizer, learning rate 1e-1 and batch size 512, for two-layer finetuning, we use the learning rate 10^{-2} and batch size 512.

B.2 Additional Experimental Results

Table 5 showcases the effectiveness of RPVopt on the CIFAR10 dataset with CLIP backbone. Overall, RPVopt achieves superior performance in terms of F1 and accuracy scores compared to other baselines. Notably, at the smallest coreset size, our proposed method outperforms other baselines by large margins. Across all setups, RPVopt either achieves the best performance or is comparable to the top-performing method, further confirming the robustness and effectiveness of RPVopt.

| Method | Metric | 50 | 100 | 200 | 500 | 1000 | 1500 | 2000 | 2500 | 3000 | 3500 | 4000 |
|---|--------|------------------------------------|------------------------------------|------------------------------------|------------------------------------|------------------------------------|------------------------------------|------------------------------------|------------------------------------|------------------------------------|------------------------------------|------------------------------------|
| 11-16 | Acc | 79.82 ± 2.06 | 88.51 ± 0.44 | 90.90 ± 0.13 | $\textbf{92.47} \pm \textbf{0.12}$ | $\textbf{93.00} \pm \textbf{0.07}$ | 93.23 ± 0.08 | 93.39 ± 0.06 | 93.57 ± 0.03 | $\textbf{93.68} \pm \textbf{0.05}$ | 93.72 ± 0.05 | $\textbf{93.80} \pm \textbf{0.04}$ |
| Method Uniform Herding [47] Contextual Diversity [51] Glister [52] GraNd [53] Forgetting [54] DeepFool [55] Entropy [56] Margin [56] LeastConfidence [56] RPVopt | F1 | 78.41 ± 2.72 | 88.56 ± 0.45 | 90.92 ± 0.12 | $\textbf{92.47} \pm \textbf{0.12}$ | $\textbf{93.00} \pm \textbf{0.07}$ | 93.24 ± 0.08 | 93.40 ± 0.06 | 93.58 ± 0.03 | $\textbf{93.69} \pm \textbf{0.05}$ | 93.73 ± 0.05 | $\textbf{93.82} \pm \textbf{0.04}$ |
| Herding [47] | Acc | 86.09 ± 0.34 | 88.21 ± 0.54 | 90.77 ± 0.15 | 91.81 ± 0.20 | 92.73 ± 0.08 | 93.10 ± 0.06 | 93.34 ± 0.02 | 93.34 ± 0.08 | 93.60 ± 0.07 | 93.76 ± 0.04 | 93.67 ± 0.06 |
| ficiality [47] | Fl | 86.29 ± 0.33 | 88.36 ± 0.52 | 90.81 ± 0.14 | 91.83 ± 0.19 | 92.74 ± 0.08 | 93.11 ± 0.06 | 93.35 ± 0.02 | 93.35 ± 0.08 | 93.61 ± 0.07 | 93.78 ± 0.04 | 93.69 ± 0.06 |
| Contactual Dispersity [51] | Acc | 82.76 ± 1.00 | 88.96 ± 0.34 | 90.98 ± 0.25 | 92.10 ± 0.19 | 92.69 ± 0.10 | 93.09 ± 0.07 | 93.30 ± 0.06 | 93.46 ± 0.04 | 93.58 ± 0.03 | 93.61 ± 0.03 | 93.77 ± 0.06 |
| Contextual Diversity [51] | Fl | 82.68 ± 1.16 | 89.01 ± 0.34 | 91.01 ± 0.24 | 92.12 ± 0.18 | 92.70 ± 0.10 | 93.09 ± 0.07 | 93.30 ± 0.06 | 93.45 ± 0.04 | 93.58 ± 0.03 | 93.61 ± 0.03 | 93.77 ± 0.06 |
| Glister [52] | Acc | 82.19 ± 2.00 | 88.37 ± 0.36 | 90.96 ± 0.30 | 92.41 ± 0.20 | 92.97 ± 0.10 | $\textbf{93.30} \pm \textbf{0.07}$ | 93.42 ± 0.09 | 93.58 ± 0.06 | 93.66 ± 0.06 | 93.70 ± 0.03 | 93.80 ± 0.04 |
| Glister [52] | Fl | 81.79 ± 2.33 | 88.45 ± 0.37 | 91.01 ± 0.29 | 92.41 ± 0.19 | 92.96 ± 0.10 | $\textbf{93.31} \pm \textbf{0.07}$ | 93.42 ± 0.09 | 93.59 ± 0.07 | 93.68 ± 0.06 | 93.71 ± 0.03 | 93.80 ± 0.05 |
| GroNd [52] | Acc | 82.44 ± 0.30 | 88.98 ± 0.04 | 90.38 ± 0.02 | 92.50 ± 0.03 | 92.90 ± 0.02 | 93.24 ± 0.02 | 93.38 ± 0.02 | 93.56 ± 0.02 | 93.56 ± 0.02 | 93.70 ± 0.03 | 93.77 ± 0.03 |
| Glaive [55] | Fl | 82.30 ± 0.33 | 88.87 ± 0.04 | 90.38 ± 0.03 | 92.49 ± 0.03 | 92.92 ± 0.02 | 93.26 ± 0.02 | 93.39 ± 0.02 | 93.57 ± 0.02 | 93.57 ± 0.02 | 93.71 ± 0.03 | 93.79 ± 0.03 |
| Econociting [54] | Acc | 82.16 ± 0.80 | 87.84 ± 0.67 | 90.28 ± 0.23 | 91.67 ± 0.16 | 92.90 ± 0.06 | 93.09 ± 0.06 | 93.23 ± 0.05 | 93.41 ± 0.04 | 93.50 ± 0.05 | 93.62 ± 0.02 | 93.70 ± 0.05 |
| Forgetting [54] | F1 | 82.02 ± 0.92 | 87.90 ± 0.65 | 90.30 ± 0.22 | 91.67 ± 0.16 | 92.90 ± 0.06 | 93.08 ± 0.05 | 93.23 ± 0.05 | 93.40 ± 0.04 | 93.50 ± 0.05 | 93.62 ± 0.02 | 93.71 ± 0.05 |
| DeepFool [55] | Acc | 81.50 ± 1.20 | 88.15 ± 0.33 | 90.89 ± 0.16 | 92.20 ± 0.11 | 93.07 ± 0.06 | 93.29 ± 0.06 | 93.39 ± 0.04 | 93.61 ± 0.04 | 93.65 ± 0.03 | 93.75 ± 0.04 | 93.79 ± 0.05 |
| DeepFool [55] | F1 | 80.91 ± 1.48 | 88.08 ± 0.32 | 90.87 ± 0.18 | 92.19 ± 0.11 | 93.07 ± 0.06 | 93.29 ± 0.06 | 93.39 ± 0.04 | 93.61 ± 0.04 | 93.65 ± 0.03 | 93.75 ± 0.05 | 93.80 ± 0.05 |
| Entrony [56] | Acc | 76.86 ± 0.26 | 82.32 ± 0.54 | 90.02 ± 0.05 | 92.08 ± 0.09 | 92.99 ± 0.02 | 93.09 ± 0.04 | 93.28 ± 0.04 | 93.42 ± 0.02 | 93.51 ± 0.04 | 93.62 ± 0.03 | 93.70 ± 0.01 |
| Entropy [50] | F1 | 75.19 ± 0.32 | 81.64 ± 0.67 | 90.07 ± 0.04 | 92.10 ± 0.08 | 92.99 ± 0.02 | 93.10 ± 0.04 | 93.28 ± 0.04 | 93.43 ± 0.02 | 93.52 ± 0.04 | 93.63 ± 0.04 | 93.71 ± 0.01 |
| Morain [56] | Acc | 77.06 ± 0.52 | 87.08 ± 0.48 | 89.35 ± 0.12 | 92.11 ± 0.04 | 92.95 ± 0.05 | 93.13 ± 0.03 | 93.27 ± 0.03 | 93.48 ± 0.06 | 93.47 ± 0.04 | 93.59 ± 0.03 | 93.73 ± 0.04 |
| Margin [50] | Fl | 76.05 ± 0.58 | 87.10 ± 0.52 | 89.43 ± 0.12 | 92.13 ± 0.04 | 92.97 ± 0.05 | 93.13 ± 0.03 | 93.28 ± 0.03 | 93.49 ± 0.06 | 93.48 ± 0.04 | 93.60 ± 0.03 | 93.74 ± 0.04 |
| LoostConfidence [56] | Acc | 77.35 ± 0.18 | 84.46 ± 0.15 | 90.27 ± 0.20 | 92.09 ± 0.06 | 92.85 ± 0.04 | 93.27 ± 0.03 | 93.44 ± 0.03 | 93.56 ± 0.04 | 93.60 ± 0.03 | 93.57 ± 0.02 | 93.58 ± 0.04 |
| LeastConfidence [56] | Fl | 76.24 ± 0.19 | 84.42 ± 0.16 | 90.31 ± 0.19 | 92.11 ± 0.06 | 92.86 ± 0.04 | 93.27 ± 0.03 | 93.44 ± 0.03 | 93.58 ± 0.04 | 93.61 ± 0.03 | 93.58 ± 0.03 | 93.59 ± 0.04 |
| BBVont | Acc | $\textbf{86.09} \pm \textbf{0.34}$ | $\textbf{88.98} \pm \textbf{0.04}$ | $\textbf{90.96} \pm \textbf{0.30}$ | 92.41 ± 0.20 | 92.97 ± 0.10 | 93.24 ± 0.02 | $\textbf{93.44} \pm \textbf{0.03}$ | $\textbf{93.61} \pm \textbf{0.04}$ | 93.66 ± 0.06 | $\textbf{93.75} \pm \textbf{0.04}$ | $\textbf{93.80} \pm \textbf{0.04}$ |
| KF vopt | Fl | $\textbf{86.29} \pm \textbf{0.33}$ | $\textbf{88.87} \pm \textbf{0.04}$ | $\textbf{91.01} \pm \textbf{0.29}$ | 92.41 ± 0.19 | 92.96 ± 0.10 | 93.26 ± 0.02 | $\textbf{93.44} \pm \textbf{0.03}$ | $\textbf{93.61} \pm \textbf{0.04}$ | 93.68 ± 0.06 | $\textbf{93.75} \pm \textbf{0.05}$ | 93.80 ± 0.05 |

Table 5: CIFAR10 with CLIP Linear Probing. Best results are highlighted in **bold**, standard errors with 5 random seeds. Different columns indicate different core set sizes.

Table 6: Performance of baselines on CIFAR10 when finetuning the last two layers of ResNet18.

| Method | Metric | 50 | 100 | 200 | 500 | 1000 | 1500 | 2000 | 2500 | 3000 | 3500 | 4000 |
|---------------------------|--------|------------------------------------|------------------------------------|------------------------------------|------------------------------------|------------------|------------------------------------|------------------------------------|------------------------------------|------------------------------------|------------------------------------|------------------------------------|
| Uniform Compling | Acc | 44.56 ± 0.85 | 55.30 ± 0.50 | 62.90 ± 0.42 | 70.56 ± 0.24 | 74.18 ± 0.23 | 75.90 ± 0.15 | 76.90 ± 0.21 | 77.83 ± 0.09 | $\textbf{78.39} \pm \textbf{0.12}$ | 78.29 ± 0.20 | $\textbf{78.92} \pm \textbf{0.06}$ |
| Chilofin Sampling | Fl | 40.82 ± 1.74 | 53.60 ± 0.69 | 62.38 ± 0.49 | 70.44 ± 0.28 | 74.12 ± 0.25 | 75.80 ± 0.18 | 76.83 ± 0.23 | 77.76 ± 0.10 | 78.34 ± 0.11 | 78.25 ± 0.20 | $\textbf{78.85} \pm \textbf{0.05}$ |
| Hording [47] | Acc | 40.20 ± 1.75 | 53.06 ± 1.46 | 62.35 ± 0.35 | 70.25 ± 0.25 | 73.96 ± 0.22 | 75.59 ± 0.10 | 76.46 ± 0.20 | 77.40 ± 0.20 | 77.73 ± 0.13 | 78.27 ± 0.20 | 78.57 ± 0.09 |
| fierding [47] | Fl | 35.68 ± 2.39 | 51.34 ± 1.87 | 61.79 ± 0.31 | 69.93 ± 0.40 | 73.83 ± 0.23 | 75.46 ± 0.09 | 76.37 ± 0.21 | 77.27 ± 0.21 | 77.67 ± 0.12 | 78.22 ± 0.18 | 78.52 ± 0.11 |
| Contextual Diversity [51] | Acc | 46.09 ± 1.07 | 54.57 ± 0.78 | 62.21 ± 0.27 | 70.54 ± 0.36 | 74.36 ± 0.29 | 75.75 ± 0.18 | 76.79 ± 0.15 | 77.34 ± 0.15 | 77.90 ± 0.13 | 78.48 ± 0.13 | 78.69 ± 0.17 |
| Contextual Diversity [51] | Fl | 42.55 ± 1.14 | 52.99 ± 0.88 | 61.51 ± 0.48 | 70.27 ± 0.35 | 74.24 ± 0.33 | 75.67 ± 0.19 | 76.71 ± 0.15 | 77.19 ± 0.14 | 77.75 ± 0.14 | 78.38 ± 0.15 | 78.57 ± 0.16 |
| Glietar [52] | Acc | 44.33 ± 1.71 | 53.32 ± 1.13 | 62.15 ± 0.65 | 69.77 ± 0.20 | 74.05 ± 0.20 | 75.63 ± 0.19 | 76.60 ± 0.09 | 77.48 ± 0.14 | 77.97 ± 0.07 | 78.22 ± 0.16 | 78.32 ± 0.15 |
| Glister [52] | Fl | 41.92 ± 2.16 | 51.81 ± 1.29 | 61.80 ± 0.61 | 69.64 ± 0.19 | 73.95 ± 0.20 | 75.55 ± 0.20 | 76.52 ± 0.08 | 77.40 ± 0.12 | 77.89 ± 0.08 | 78.18 ± 0.16 | 78.21 ± 0.15 |
| GraNd [53] | Acc | 42.73 ± 0.76 | 53.58 ± 1.14 | 63.30 ± 0.54 | 70.30 ± 0.03 | 74.03 ± 0.10 | 75.40 ± 0.03 | 76.42 ± 0.08 | 77.32 ± 0.26 | 77.79 ± 0.13 | 77.94 ± 0.13 | 78.50 ± 0.16 |
| 01a140 [55] | Fl | 39.02 ± 1.15 | 51.82 ± 1.63 | 63.04 ± 0.57 | 70.17 ± 0.07 | 73.90 ± 0.11 | 75.30 ± 0.03 | 76.34 ± 0.08 | 77.28 ± 0.27 | 77.74 ± 0.14 | 77.93 ± 0.10 | 78.40 ± 0.16 |
| Forgetting [54] | Acc | 43.16 ± 1.78 | 53.58 ± 1.48 | 63.07 ± 0.45 | 70.75 ± 0.23 | 73.74 ± 0.16 | 75.25 ± 0.26 | 76.24 ± 0.12 | 77.36 ± 0.10 | 77.92 ± 0.18 | 78.07 ± 0.12 | 78.41 ± 0.12 |
| r orgenning [54] | Fl | 40.55 ± 1.26 | 53.06 ± 1.59 | 62.47 ± 0.38 | 70.55 ± 0.28 | 73.60 ± 0.16 | 75.13 ± 0.26 | 76.10 ± 0.08 | 77.26 ± 0.15 | 77.85 ± 0.17 | 77.95 ± 0.10 | 78.31 ± 0.08 |
| DeenFool [55] | Acc | 43.88 ± 0.46 | 55.51 ± 0.65 | 63.05 ± 0.64 | 70.53 ± 0.27 | 73.85 ± 0.16 | 75.60 ± 0.18 | 76.54 ± 0.17 | 77.21 ± 0.17 | 77.77 ± 0.13 | 77.99 ± 0.13 | 78.39 ± 0.10 |
| Deepi 001 [55] | Fl | 40.64 ± 0.99 | 54.07 ± 0.13 | 62.62 ± 0.66 | 70.33 ± 0.31 | 73.74 ± 0.19 | 75.50 ± 0.19 | 76.41 ± 0.16 | 77.10 ± 0.17 | 77.69 ± 0.13 | 77.91 ± 0.15 | 78.29 ± 0.11 |
| Entropy [56] | Acc | 44.49 ± 1.03 | 54.20 ± 1.47 | 63.72 ± 0.40 | 70.61 ± 0.08 | 74.47 ± 0.14 | 75.66 ± 0.06 | 76.66 ± 0.15 | 77.53 ± 0.32 | 78.09 ± 0.14 | 78.22 ± 0.02 | 78.60 ± 0.13 |
| Endopy [50] | Fl | 41.64 ± 1.36 | 52.14 ± 1.41 | 63.24 ± 0.44 | 70.30 ± 0.20 | 74.34 ± 0.16 | 75.55 ± 0.05 | 76.57 ± 0.14 | 77.47 ± 0.32 | 78.04 ± 0.15 | 78.17 ± 0.02 | 78.52 ± 0.13 |
| Margin [56] | Acc | 43.67 ± 0.55 | 53.50 ± 1.70 | 62.67 ± 0.44 | 70.80 ± 0.29 | 74.75 ± 0.16 | 75.71 ± 0.14 | 76.58 ± 0.16 | 77.71 ± 0.17 | 78.11 ± 0.22 | 78.25 ± 0.12 | 78.63 ± 0.22 |
| Margin [50] | Fl | 41.37 ± 1.29 | 51.50 ± 1.93 | 62.12 ± 0.34 | 70.49 ± 0.35 | 74.64 ± 0.18 | 75.59 ± 0.13 | 76.49 ± 0.14 | 77.67 ± 0.18 | 78.02 ± 0.23 | 78.13 ± 0.15 | 78.56 ± 0.21 |
| LoostConfidence [56] | Acc | 44.60 ± 1.74 | 53.94 ± 0.70 | 62.56 ± 0.53 | $\textbf{70.91} \pm \textbf{0.20}$ | 74.55 ± 0.12 | $\textbf{76.28} \pm \textbf{0.10}$ | 76.68 ± 0.11 | 77.54 ± 0.23 | 78.04 ± 0.19 | 78.30 ± 0.18 | 78.78 ± 0.15 |
| LeastConfidence [50] | Fl | 40.55 ± 2.19 | 52.51 ± 1.01 | 61.97 ± 0.65 | $\textbf{70.69} \pm \textbf{0.18}$ | 74.27 ± 0.26 | $\textbf{76.13} \pm \textbf{0.10}$ | 76.63 ± 0.09 | 77.43 ± 0.22 | 77.98 ± 0.21 | 78.19 ± 0.19 | 78.73 ± 0.16 |
| RPVont | Acc | $\textbf{45.92} \pm \textbf{1.30}$ | $\textbf{55.82} \pm \textbf{0.92}$ | $\textbf{63.52} \pm \textbf{0.81}$ | 70.75 ± 0.26 | 74.53 ± 0.16 | 76.03 ± 0.29 | $\textbf{76.92} \pm \textbf{0.12}$ | $\textbf{77.90} \pm \textbf{0.17}$ | 78.19 ± 0.10 | $\textbf{78.58} \pm \textbf{0.09}$ | 78.88 ± 0.14 |
| KF vopt | Fl | 43.00 ± 1.68 | 54.33 ± 1.08 | $\textbf{63.08} \pm \textbf{1.02}$ | 70.63 ± 0.26 | 74.38 ± 0.17 | 75.89 ± 0.30 | 76.78 ± 0.15 | 77.76 ± 0.17 | 78.03 ± 0.11 | 78.46 ± 0.09 | 78.80 ± 0.13 |

Similar to the experiment in the main paper, we finetune ResNet18 by updating the weights of the last two layers only and provide the obtained scores in Table 6. Throughout our experiments, RPVopt demonstrates competitive performance, especially with large improvements observed on non-homogeneous datasets such as StanfordCars. When the sample size is small, e.g. 50 in CIFAR10 and 500 in StanfordCars, our method effectively identifies and selects informative samples that benefit downstream tasks.