Convex Hull Approximation of Nearly Optimal Lasso Solutions

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Abstract

In an ordinary feature selection procedure, a set of important features is obtained by solving an optimization problem such as the Lasso regression problem, and we expect that the obtained features explain the data well. In this study, instead of the single optimal solution, we consider finding a set of diverse yet nearly optimal solutions. To this end, we formulate the problem as finding a small number of solutions such that the convex hull of these solutions approximates the set of nearly optimal solutions. The proposed algorithm consists of two steps: First, we randomly sample the extreme points of the set of nearly optimal solutions. Then, we select a small number of points using a greedy algorithm. The experimental results indicate that the proposed algorithm can approximate the solution set well. The results also indicate that we can obtain Lasso solutions with a large diversity.

1 Introduction

Background and Motivation

Feature selection is a procedure for finding a small set of relevant features from a dataset. It simplifies the model to make them easier to understand, and enhances the generalization performance; thus it plays an important role in data mining and machine learning [Guyon and Elisseeff, 2003].

One of the most commonly used feature selection methods is the Lasso regression [Tibshirani, 1996][Chen et al., 2001]. Suppose that we have \(n\) observations of \(p\) dimensional vectors \(x_1, \ldots, x_n \in \mathbb{R}^p\), and the corresponding responses \(y_1, \ldots, y_n \in \mathbb{R}\). Then, the Lasso regression seeks a feature vector \(\beta^* \in \mathbb{R}^p\) by minimizing the \(\ell_1\)-penalized squared loss function

\[
L(\beta) = \frac{1}{2n} \|X\beta - y\|_2^2 + \lambda \|\beta\|_1, \tag{1.1}
\]

where \(X = [x_1; \cdots; x_n] \in \mathbb{R}^{n \times p}\) and \(y = [y_1; \cdots; y_n] \in \mathbb{R}^n\). Here, \(\| \cdot \|_p\) denotes the \(\ell_p\)-norm defined by \(\|\beta\|_p = (\sum_j |\beta_j|^p)^{1/p}\). Since the \(\ell_1\) penalty induces sparsity of the solution, we may obtain a set of features from the support of the solution.
Figure 1: Illustration of our approach. The triangle shows the optimal solution $B(\nu^*) = \{\beta^*\}$, the dashed line shows the boundary of the nearly optimal solutions $B(\nu)$, and the squares with the solid line show the convex hull approximation $\text{conv}(Q)$ of $B(\nu)$.

The Lasso regression and its variants have many desirable properties; in particular, the sparsity of the solution helps users to understand which features are important for their tasks. Hence, they are considered to be one of the most basic approaches for the cases, e.g., when models are used to support user decision making where the sparsity allows users to check whether or not the models are reliable; and, when users are interested in finding interesting mechanisms underlying the data where the sparsity enables users to identify important features and get insights of the data [Guyon and Elisseeff, 2003].

To further strengthen those advantages of the Lasso, Hara and Maehara [2017] proposed enumerating all (essentially different) the Lasso solutions in their increasing order of the objective values. With the enumeration, one can find more reliable models from the enumerated solutions, or one can gain more insights of the data [Hara and Maehara, 2017, Hara and Ishihata, 2018].

In this study, we aim at finding diverse solutions instead of the exhaustive enumeration. Hara and Maehara [2017] have observed that in real-world applications, there are too many nearly optimal solutions to enumerate them exhaustively. Typically, if there are some highly correlated features, the enumeration algorithm outputs all their combinations as nearly optimal solutions; thus, there are exponentially many nearly optimal solutions. Obviously, checking all those similar solutions is too exhausting for the users, which makes the existing enumeration method less practical. To overcome this practical limitation, we consider finding diverse solutions as the representative of the nearly optimal solutions, which enables users to check “overview” of the solutions.

**Contribution** In this study, we propose a novel formulation to find diverse yet nearly optimal Lasso solutions. Instead of the previous enumeration approach, we directly work on the set of nearly optimal solutions, defined by

$$B(\nu) = \{\beta \in \mathbb{R}^p : L(\beta) \leq \nu\}$$ (1.2)
where $\nu \in \mathbb{R}$ is a threshold slightly greater than the optimal objective value $\nu^* = L(\beta^*)$ of the Lasso regression.

We summarize $B(\nu)$ by a small number of points $Q \subset B(\nu)$ in the sense that the convex hull of $Q$ approximates $B(\nu)$. We call this approach convex hull approximation. Section 3 describes the mathematical formulation of our approach. We illustrate this approach in the following example with Figure 1.

**Example 1.1.** Let us consider the two-dimensional Lasso regression problem with the following loss function

$$L(\beta_1, \beta_2) = \frac{1}{2} \left\| \begin{bmatrix} 1 & 1 + \epsilon \\ 1 + \epsilon & 1 \end{bmatrix} \begin{bmatrix} \beta_1 \\ \beta_2 \end{bmatrix} - \begin{bmatrix} 1 \\ 1 \end{bmatrix} \right\|_2^2 + \left\| \begin{bmatrix} \beta_1 \\ \beta_2 \end{bmatrix} \right\|_1$$

(1.3)

where $\epsilon$ is a sufficiently small parameter, e.g., $\epsilon = 1/40$. Then, the optimal value $\nu^*$ is approximately $3/4$, and the corresponding optimal solution $\beta^*$ is approximately $(0, 1/2)$, as shown in the green point in Figure 1.

Now, we consider the nearly optimal solution set $B(\nu)$ for the threshold $\nu = \nu^* + \epsilon$. The boundary of this set is illustrated in the dashed line in Figure 1. Even if $\nu - \nu^*$ is very small, since the observations $X$ is highly correlated, $B(\nu)$ contains essentially different solution, e.g., $\beta' = (1/2, 0)$.

We approximate $B(\nu)$ by the convex hull of a few finite points $Q \subset B(\nu)$. In this case, by taking the corner points of $B(\nu)$, we can approximate this set well by the four points as shown by the blue line in Figure 1. We note that the diversity of $Q$ is implicitly enforced because diverse $Q$ is desirable for a good approximation of $B(\nu)$; we therefore do not need to add the diversity constraint such as DPP [Kulesza et al., 2012] explicitly.

This problem will be solved numerically in Section 5.

We propose an algorithm to construct a good convex hull approximation of $B(\nu)$. The algorithm consists of two steps. First, it samples sufficiently many extreme points of $B(\nu)$ by solving Lasso regressions multiple times. Second, we select a small subset $Q$ from the sampled points to yield a compact summarization. The detailed description of our algorithm is given in Section 4.

We conducted numerical experiments to evaluate the effectiveness of the proposed method. Specifically, we evaluated three aspects of the method, namely, the approximation performance, computational efficiency, and the diversity of the found solutions. The results are shown in Section 5.

For simplicity, we describe only the method for Lasso regression in the manuscript; however it can be easily adopted to the other models such as the sparse logistic regression [Lee et al., 2006] and elastic-net [Zou and Hastie, 2005].

## 2 Preliminaries

A set $C \subset \mathbb{R}^p$ is convex if for any $\beta_1, \beta_2 \in C$ and $\alpha \in [0, 1]$, $(1 - \alpha)\beta_1 + \alpha \beta_2 \in C$. For a set $P \subset \mathbb{R}^p$, its convex hull, $\text{conv}(P)$, is the smallest convex set containing $P$. Let $C$ be a convex set. A point $\beta \in C$ is an extreme point of $C$ if $\beta = (1 - \alpha)\beta_1 + \alpha \beta_2$.
for some $\beta_1, \beta_2 \in C$ and $\alpha \in (0, 1)$ implies $\beta = \beta_1 = \beta_2$. The set of extreme points of $C$ is denoted by $\text{ext}(C)$.

The Klein–Milman theorem shows the fundamental relation between the extreme points and the convex hull.

**Theorem 2.1** (Klein–Milman Theorem; see Barvinok [2002]). Let $C$ be a compact convex set. Then $\text{conv}(\text{ext}(C)) = C$.

For two sets $C, C' \subset \mathbb{R}^p$, the **Hausdorff distance** between these sets is defined by

$$d(C, C') = \max\{\sup_{\beta \in C} \inf_{\beta' \in C'} \|\beta - \beta'\|_2, \sup_{\beta' \in C'} \inf_{\beta \in C} \|\beta - \beta'\|_2\}. \quad (2.1)$$

The Hausdorff distance forms a metric on the non-empty compact sets. The computation of Hausdorff distance is NP-hard (more strongly, it is $\text{W}[1]$-hard) in general [König, 2014].

A function $L : \mathbb{R}^p \to \mathbb{R}$ is convex if the epigraph $\text{Epi}(L) = \{(\beta, \nu) \in \mathbb{R}^p \times \mathbb{R} : \nu \geq L(\beta)\}$ is convex. For a convex function $L$, the level set $B(\nu) = \{\beta \in \mathbb{R}^p : L(\beta) \leq \nu\}$ is convex for all $\nu \in \mathbb{R}$.

### 3 Formulation

In this section, we formulate our convex hull approximation problem mathematically. We assume that $X$ has no zero column (otherwise, we can remove the zero column and the corresponding feature from the model).

Recall that the Lasso loss function $L : \mathbb{R}^p \to \mathbb{R}$ in (1.1) is convex; therefore, the set of nearly optimal solutions $B(\nu)$ in (1.2) forms a closed convex set. Moreover, since $X$ has no zero column, $B(\nu)$ is compact.

Our goal is to summarize $B(\nu)$. By the Klein–Milman theorem (Theorem 2.1), $B(\nu)$ can be reconstructed from the extreme points of $B(\nu)$ as $B(\nu) = \text{conv}(\text{ext}(B(\nu)))$; therefore, it is natural to output the extreme points $\text{ext}(B(\nu))$ as a summary of $B(\nu)$. If $\nu = \nu^*$, this approach corresponds to enumerating the vertices of $B(\nu^*)$, which forms a polyhedron [Tibshirani and others, 2013]; therefore, we can use the existing algorithm to enumerate the vertices of a polyhedron developed in Computational Geometry [Fukuda et al., 1997] as in Pantazis et al. [2017]. However, if $\nu > \nu^*$, $B(\nu)$ has a piecewise smooth boundary, as shown in Figure 1; therefore, there are continuously many extreme points of $B(\nu)$, which cannot be enumerated.

Therefore, we select a finite number of points $Q \subset \text{ext}(B(\nu))$ as a “representative” of the extreme points such that $\text{conv}(Q)$ well approximates $B(\nu)$. We measure the quality of the approximation by the Hausdorff distance (2.1).

To summarize the above discussion, we pose the following problem.

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1Pantazis et al. [2017] also consider the near optimal solutions. However, they focused only on the subset of $B(\nu)$ spanned by the support of the Lasso global solution. We do not take this approach since it cannot handle a global structure of $B(\nu)$. 

4
Algorithm 1 Proposed algorithm

1: Sample sufficiently many points \( S \subset B(\nu) \) by Algorithm 2.
2: Select a few points \( Q \subseteq S \) by Algorithm 3.

Problem 3.1. We are given a loss function \( L : \mathbb{R}^p \to \mathbb{R} \) and a threshold \( \nu \in \mathbb{R} \). Let \( B(\nu) = \{ \beta \in \mathbb{R}^p : L(\beta) \leq \nu \} \). Find a point set \( Q \subset B(\nu) \) such that (1) \( d(\text{conv}(Q), B(\nu)) \) is small, and (2) \( |Q| \) is small.

The problem of approximating a convex set by a polyhedron has a long history in convex geometry (see Bronstein [2008] for a recent survey). Asymptotically, for any compact convex set with a smooth boundary, the required number of points to obtain an \( \epsilon \) approximation is \( \Theta(\sqrt{p}/\epsilon^{(p-1)/2}) \) [Bronstein and Ivanov, 1975, Gruber, 1993]. Therefore, in the worst case, we may need exponentially many points to have a reasonable approximation.

On the other hand, if we focus on the non-asymptotic \( \epsilon \), we have a chance to obtain a simple representation. One intuitive situation is that the polytope \( B(\nu^*) \) has a small number of vertices, as in Figure 1. In such a case, by taking the vertices as \( Q \), we can obtain an \( O(\epsilon) \) approximation for \( B(\nu) \) when \( \nu = \nu^* + O(\epsilon) \).

Therefore, below, we assume that \( B(\nu) \) admits a small number of representatives and construct an algorithm to find such representatives.

4 Algorithm

In this section, we propose a method to compute a convex hull approximation \( \text{conv}(Q) \) of \( B(\nu) \).

Since \( \text{conv}(Q) \subseteq B(\nu) \) and the sets are compact, the Hausdorff distance between \( \text{conv}(Q) \) and \( B(\nu) \) is given by

\[
d(\text{conv}(Q), B(\nu)) = \max_{\beta \in B(\nu)} \min_{\beta' \in \text{conv}(Q)} \| \beta - \beta' \|_2.
\]

(4.1)

A natural approach is to minimize this quantity by a greedy algorithm that successively selects the maximizer \( \beta \in B(\nu) \) of (4.1) and then adds it to \( Q \). However, this approach is impractical, because the optimization problem (4.1) is a convex maximization problem.

To overcome this difficulty, we use a random sampling approximation for \( B(\nu) \). We first sample sufficiently many points \( S \) from \( \text{ext}(B(\nu)) \) and then regard \( \text{conv}(S) \) as an approximation of \( B(\nu) \). Once this approximation is constructed, the maximum in (4.1) can be obtained by a simple linear search. Therefore, this reduces our problem to a simple subset selection problem.

The overall procedure of our algorithm is shown in Algorithm 1. It consists of two steps: random sampling step and subset selection step. Below, we describe each step.

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2In our preliminary study, we implemented the projected gradient method to find the farthest point \( \beta \in B(\nu) \). However, it was slow, and often converged to poor local maximal solutions.
Algorithm 2 Sampling points

1: \( S = \emptyset \)
2: for \( j = 1, 2, \ldots, M \) do
3: \( \text{Draw } d \sim N(0, I) \)
4: Solve (4.2) to obtain an extreme point \( \beta(d) \) and add it to \( S \)
5: end for
6: Return \( S \)

4.1 Sampling Extreme Points (Algorithm 2)

Figure 1 suggests that selecting corner points of \( B(\nu) \) as \( Q \) is desirable to obtain a good approximation of \( B(\nu) \). Here, to obtain a good candidate of \( Q \), we consider a sampling algorithm that samples the corner points of \( B(\nu) \).

First, we select a uniformly random direction \( d \in \mathbb{R}^p \). Then, we find the extreme point \( \beta \in B(\nu) \) by solving the following problem

\[
\max \{ d^T \beta : \beta \in B(\nu) \}. \tag{4.2}
\]

We solve this problem by using the Lagrange dual with binary search as follows. With the Lagrange duality, we obtain the following equivalent problem

\[
\min_{\tau \geq 0} D(\tau | d) := \max_{\beta} \left( d^T \beta - \tau(L(\beta) - \nu) \right). \tag{4.3}
\]

Since the optimal solution \( \beta(d) \) of (4.2) satisfies \( L(\beta(d)) = \nu \), we seek \( \tau \) by using a binary search\(^3\) so that \( L(\beta(d)) = \nu \) to hold.

It should be noted that the proposed sampling algorithm can be completely parallelized.

Properties of Sampling The solution to the problem (4.2) tends to be sparse because of the \( \ell_1 \) term in \( L(\beta) \), which indicates that we can sample a corner point of \( B(\nu) \) in the direction of \( d \), such as the ones in Figure 1. More precisely, the proposed algorithm samples each extreme point with probability proportional to the volume of the normal cone of each point. Because the corner points have positive volumes, the algorithm samples corner points with high probabilities.

4.2 Greedy Subset Selection (Algorithm 3)

Next, we select a small subset \( Q \subseteq S \) from the sampled points \( S \subset \mathbb{R}^p \) that do not lose the approximation quality.

We use the farthest point selection method, proposed in Blum et al. 2016.\(^4\) In this procedure, we start from any point \( \beta_1 \in S \). Then, we iteratively select the point \( \beta_j \in S \) by solving the sample-approximated version of (4.1), i.e., the farthest point from the

\(^3\)Since we have no upper bound of the search range, we actually use the exponential search that successively doubles the search range [Bentley and Yao, 1976].

\(^4\)Blum et al. 2016 called this procedure Greedy Clustering.
Algorithm 3 Select points

1: Select $\beta_1 \in S$ arbitrary and let $Q = \{\beta_1\}$
2: Initialize a heap data structure $H$ by $H[\beta] \leftarrow d(\beta, Q)$ for all $\beta \in S \setminus Q$
3: while $|Q| < K$ do
4: Let $\beta \in H$ be the point that has the largest $H[\beta]$
5: Update $H[\beta] \leftarrow d(\beta, Q)$
6: if $H[\beta]$ is still the largest point then
7: Add $\beta$ to $Q$ and remove $\beta$ from the heap
8: end if
9: end while
10: Output $Q$

convex hull is taken as

$$\beta_j \in \arg \max_{\beta \in S} \min_{\beta' \in \text{conv}\{\beta_1, \ldots, \beta_{j-1}\}} \|\beta - \beta'\|_2.$$ \hfill (4.4)

This procedure has the following theoretical guarantee.

**Theorem 4.1** (Blum et al. [2016]). Let $S \subset \mathbb{R}^p$ be a finite set enclosed in the unit ball. Suppose that there exists a finite set $Q^* \subset S$ of size $k^*$ such that $d(\text{conv}(Q^*), \text{conv}(S)) \leq \epsilon$. Then, the greedy algorithm finds a set $Q \subset S$ of size $k^*/\epsilon^{2/3}$ with $d(\text{conv}(Q), \text{conv}(S)) = O(\epsilon^{1/3}).$

Thus, if the number of samples $|S|$ are sufficiently large such that $d(\text{conv}(S), B(\nu)) \leq \epsilon$, the algorithm finds a convex hull approximation with $O(\epsilon^{1/3})$ error.

Below, we describe how to implement this procedure. First, the distance from $\beta$ to the convex hull of $\beta_1, \ldots, \beta_k$ is computed by solving the following problem:

$$\min_{\alpha} \|\beta - \sum_j \alpha_j \beta_j\|^2$$
$$\text{s.t. } \sum_j \alpha_j = 1, \alpha_j \geq 0.$$ \hfill (4.5)

This problem is a convex quadratic programming problem, which can be solved efficiently by using the interior point method [Achache, 2006].

To implement the greedy algorithm, we have to evaluate the distance from each point to the current convex hull. However, this procedure can be expensive when $|S|$ is large as we need to solve the problem (4.5) many times. For efficient computation, we need to avoid evaluating the distance as much as possible.

We observe that, if we add a new point $\beta_j$ to the current convex hull, the distances from other points to the convex hull decrease monotonically. Therefore, we can use the lazy update technique [Minoux, 1978] to accelerate the procedure as follows.

We maintain the points $S$ by a heap data structure whose keys are the upper bounds of the distance to the convex hull. First, we select an arbitrary point $\beta_1$, and then initialize the key of $\beta \in S$ by $d(\beta_1, \beta)$. For each step, we select the point $\beta'_j \in S$ from the heap such that $\beta'_j$ has the largest distance upper bound. Then, we recompute the distance $d(\beta'_j, \text{conv}(Q))$ by solving the quadratic program (4.5) and update the key of
If it still has the largest distance upper bound, it is the farthest point; therefore, we select $\beta'_j$ as the $j$-th point $\beta_j$. Otherwise, we repeat this procedure until we find the farthest point. See Algorithm 3 for the detail.

5 Experiments

We evaluate the three aspects of the proposed algorithm, namely, the approximation performance, computational efficiency, and the diversity of the found solutions. First, we visualize the results of the algorithm by using a low dimensional synthetic data (Section 5.1). Then, we evaluate the approximation performance and computational efficiency by using a larger dimensional synthetic data (Sections 5.2 and 5.3). Finally, we evaluate the diversity of the obtained solutions by using real-world datasets (Section 5.4 and 5.5).

Sample Approximation of Hausdorff Distance for Evaluation

We evaluate the approximation performance by the Hausdorff distance between the obtained convex hull and $B(\nu)$. However, the exact Hausdorff distance cannot be computed since it requires solving a convex maximization problem. We therefore adopt the sample approximation of Hausdorff distance, which is derived as follows:

1. Sample $M'$ extreme points $Q^*$ by using Algorithm 2.
2. Define the sample approximation of $B(\nu)$ by the convex hull $\text{conv}(Q^*)$.
3. Measure the Hausdorff distance $d(\text{conv}(Q), \text{conv}(Q^*))$ as an approximation of $d(\text{conv}(Q), B(\nu))$.

Implementations

The codes were implemented in Python 3.6. In Algorithm 2 to solve the problem (4.3), we used enet_coordinate_descent_gram function in scikit-learn. In Algorithm 3, we selected the first point $\beta_1 \in S$ as $\beta_1 = \arg\max_{\beta \in S} \|\beta - \beta^*\|_2$. To compute the projection (4.5), we used CVXOPT library. The experiments were conducted on a system with an Intel Xeon E5-1650 3.6GHz CPU and 64GB RAM, running 64-bit Ubuntu 16.04.

5.1 Visual Demonstration

For visual demonstration, we consider two examples: Example 1.1 in Section 1 and Example 5.1 defined below.

Example 5.1. Consider the three-dimensional Lasso regression problem with the following loss function

$$L(\beta) = \frac{1}{2} \left\| \begin{bmatrix} 1 & 1 & 1 \\ 1 & 1 + \epsilon & 1 \\ 1 & 1 & 1 + 2\epsilon \end{bmatrix} \begin{bmatrix} \beta_1 \\ \beta_2 \\ \beta_3 \end{bmatrix} - \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix} \right\|^2_2 + \|\beta_1\|_1$$

(5.1)
where $\epsilon$ is a sufficiently small parameter. Then, the optimal value $\nu^*$ is approximately $5/6$, and the corresponding optimal solution $\beta^*$ is approximately $(0, 0, 2/3)$. We set $\epsilon = 1/40$, and define the set $B(\nu)$ by $\nu = 5/6 + \epsilon$.

In Example 1.1 because of the correlation between the two features, there exists a nearly optimal solution $\beta = (1/2, 0)$, apart from the optimal solution $\beta^* = (0, 1/2)$. The objective of the proposed method is therefore to find a convex hull that covers these solutions. Similarly, in Example 5.1 three features are highly correlated. The objective is to find a convex hull that covers nearly optimal solutions such as $\beta = (2/3, 0, 0)$, $(0, 2/3, 0)$, and $(0, 0, 2/3)$.

Figure 2 and 3 show the results of the proposed method for the examples. Here, we set the number of samples $M$ in Algorithm 2 to be 50, and the number of greedy point selection selection $K = |Q|$ in Algorithm 3 to be four and six, respectively. Figures 2(a) and 2(b) show that the proposed method successfully approximated $B(\nu)$ by using a few points. Indeed, as shown in Figure 3, the approximation errors converged to almost zeros indicating that $B(\nu)$ is well-approximated with convex hulls.

### 5.2 Approximation Performance

We now turn to exhaustive experiments to verify the performance of the proposed algorithm in general settings. Specifically, we show that the proposed algorithm can approximate $B(\nu)$ well, even in higher dimensions.

We generate higher dimensional data by

$$x \sim \mathcal{N}(0_p, \Sigma), \quad y = x^T \beta + \varepsilon, \quad \varepsilon \sim \mathcal{N}(0, 0.01),$$  

(5.2)

where $\Sigma_{ij} = \exp(-0.1|i - j|)$, and $\beta_i = 10/p$ if $\text{mod}(i - 1, 10) = 0$ and $\beta_i = 0$ otherwise. Because of the correlations induced by $\Sigma$, the neighboring features in $x$ are highly correlated, which indicates that there may exist several nearly optimal $\beta$. 
Figure 3: Approximation errors of $B(\nu)$, measured by the Hausdorff distance ($M' = 1,000$).

We set the number of observations $n$ to be $p = 2n$, and the regularization parameter $\lambda$ to be 0.1. We also define the set $B(\nu)$ by setting $\nu = 1.01L(\beta^*)$.

Figure 4 is the result for $p = 100$. The figure shows that the proposed algorithm can approximate $B(\nu)$ well. In the figure, there are two important observations. First, as the number of samplings $M$ increases, the Hausdorff distance decreases, indicating that the approximation performance improves. This result is intuitive in that a many greater number of candidate points lead to a better approximation.

Second, the choice of the number of samplings $M$ is not that fatal in practice. The result shows that the difference between the Hausdorff distances for $M = 200$ and for $M = 10,000$ is subtle. It also shows that the the Hausdorff distance for $M = 1,000$ and for $M = 10,000$ are almost identical for larger $K$. This indicates that we do not have to sample many points in practice.

5.3 Computational Efficiency

Next, we evaluate the computational efficiency by using the same setting (5.2) used in the previous section.

Table 1 shows the runtimes of the proposed method for $p = 100$ and $p = 1,000$ by fixing $K = 100$. The computational time for the sampling step increases as the number of samples $M$ and the dimension $p$ increases. Since the approximation performance does not improve so much as the number of samples $M$ increases as observed in the previous experiment, it is helpful in practice to use a moderate number of samples. The computational time for the greedy selection step also increases as the number of samples $M$ increases; however, interestingly, it decreases as the dimension $p$ increases. This reason is understood by observing the number of distance evaluations as follows.

Figure 5 shows the number of distance evaluations in the greedy selection step in each $K$. This shows that the redundant distance computation is significantly reduced.
Table 1: Runtime (in sec.) of the proposed algorithm (Sampling: Algorithm 2, Greedy: Algorithm 3) for selecting $K = 100$ vertices over the numbers of samples $M = 1,000, 10,000$, and 100,000.

| $M$      | $p = 100$ Sampling | $p = 100$ Greedy | $p = 1,000$ Sampling | $p = 1,000$ Greedy |
|----------|-------------------|-----------------|----------------------|-------------------|
| 1,000    | 2.891             | 34.87           | 46.54                | 17.99             |
| 10,000   | 27.80             | 178.5           | 2466                 | 66.95             |
| 100,000  | 279.1             | 1548            | 4586                 | 379.9             |

by the lazy update technique; therefore Algorithm 3 only performs a few distance evaluation in each iteration. In particular, for $p = 1,000$, the saturation is very sharp; thus the computational cost is significantly reduced. This may be because, in high-dimensional problems, adding one point to the current convex hull does not change the distance to the remaining points, and hence the lazy update helps to avoid most of distance evaluations.

5.4 Diversity of Solutions

One of the practical advantages of the proposed method is that it can find nearly optimal solutions with a large diversity. This is a favorable property when one is interested in finding several possible explanations for a given data, which is usually the case in data mining.
Setup. Here, we verify the diversity of the found solutions on the 20 Newsgroups data\footnote{http://qwone.com/˜jason/20Newsgroups/}. The results on other datasets can be found in the next section. In this experiment, we consider classifying the documents between the two categories ibm.pc.hardware and mac.hardware. As a feature vector $x$, we used tf-idf weighted bag-of-words expression, with stop words removed. The dataset comprised $n = 1,168$ samples with $p = 11,648$ words. Our objective is to find discriminative words that are relevant to the classification of the documents.

Because the task is binary classification with $y \in \{-1, +1\}$, instead of the squared objective, we use the Lasso logistic regression with the objective function given as

$$L(\beta) = \frac{1}{n} \sum_{i=1}^{n} \log(1 + \exp(-y_i x_i^\top \beta)) + \lambda \|\beta\|_1.$$  \hfill (5.3)

We implemented the solver for the problem (5.3) by modifying liblinear \cite{Fan et al., 2008}. In the experiment, we set the regularization parameter $\lambda$ to be 0.001.

Baseline Methods. We compared the solution diversity of the proposed method with the two baselines in Hara and Maehara \cite{2017}. The first baseline simply enumerates the optimal solutions with different supports in the ascending order of the objective function value (5.3). We refer to this method as Enumeration. The second baseline employs a heuristic to skip similar solutions during the enumeration. It can therefore improve the diversity of the enumerated solutions. We refer to this heuristic method as Heuristic. Note that we did not adopt the method of Pantazis et al. \cite{2017} as the baseline because it enumerates only the sub-support of the Lasso global solution: it cannot find solutions apart from the global solution.

Result. With each method, we found 500 nearly optimal $\beta$, and summarized the result in Figure 6. For the proposed method, we defined $B(\nu)$ by $\nu = 1.05L(\beta^*)$, and set the number of samplings $M$ to be 10,000. To draw the figure, we used PCA and

![Figure 5: # of distance evaluations in Algorithm 3](image-url)
Figure 6: Found 500 solutions in 20 Newsgroups data, shown in 2D using PCA.

Table 2: Representative words found in 20 Newsgroups data

| Enumeration | Heuristic | Proposed |
|-------------|-----------|----------|
| “apple”     | ✓         | ✓        | ✓        |
| “macs”      | ✗         | ✓        | ✓        |
| “macintosh” | ✗         | ✗        | ✓        |

We also note that the proposed method found 889 words in total within the 500 models. This is contrastive to Enumeration and Heuristic where they found only 39 and 63 words, respectively, which is more than ten times less than the proposed method. Table 2 shows some representative words found in 20 Newsgroups data. As the word “apple” is strongly related to the documents in mac.hardware, it is found by all the methods. However, although “macs” and “macintosh” are also relevant to mac.hardware, “mac” is overlooked by Enumeration, and “macintosh” is found only by the proposed method. This result also suggests that the proposed method can induce a large diversity and it can avoid overlooking informative features.

We note that the Lasso global solution attained 81% test accuracy, while the found 500 solutions attained from 77% to 83% test accuracies. This result indicates that the proposed method could find solutions with almost equal qualities while inducing solution diversities.
Here, we present the results on some of libsvm datasets: we used cputime for regression, and australian, german.numer, ionosphere, sonar, and splice for binary classification. In the experiments, we searched for 50 near optimal solutions using the proposed method where we set $\nu = 1.05L(\beta^*)$ and the number of samplings $M = 1,000$. We also enumerated 50 solutions using the two baselines, Enumeration and Heuristics.

The results are shown in Figure 7. For regression, we set $\rho = 0.1$, and for binary classification, we set $\rho = 0.01$, so that the solutions to be sufficiently sparse. In the figures, similar to the results in Section 5.4, we have projected the solutions into two dimensional space using PCA. The figures show the clear advantage of the proposed method in that it can find solutions with large diversities compared to the exhaustive enumerations.

### 6 Conclusion

In this study, we considered a convex hull approximation problem that seeks a small number of points such that their convex hull approximates the nearly optimal solution set to the Lasso regression problem. We propose an algorithm to solve this problem. The algorithm first approximates the nearly optimal solution set by using the convex hull of sufficiently many points. Then, it selects a few relevant points to approximate the convex hull. The experimental results indicate that the proposed method can find diverse yet nearly optimal solutions efficiently.

[6] https://www.csie.ntu.edu.tw/~cjlin/libsvmtools/datasets/
References

Mohamed Achache. A new primal-dual path-following method for convex quadratic programming. *Computational & Applied Mathematics*, 25(1):97–110, 2006.

Alexander Barvinok. *A course in convexity*, volume 54. American Mathematical Society Providence, RI, 2002.

Jon Louis Bentley and Andrew Chi-Chih Yao. An almost optimal algorithm for unbounded searching. *Information Processing Letters*, 5(3):82–87, 1976.

Avrim Blum, Sariel Har-Peled, and Benjamin Raichel. Sparse approximation via generating point sets. In *Proceedings of the Twenty-Seventh Annual ACM-SIAM Symposium on Discrete Algorithms*, pages 548–557. Society for Industrial and Applied Mathematics, 2016.

Efim M Bronstein and L. D. Ivanov. The approximation of convex sets by polyhedra. *Siberian Mathematical Journal*, 16(5):852–853, 1975.

Efim M Bronstein. Approximation of convex sets by polytopes. *Journal of Mathematical Sciences*, 153(6):727–762, 2008.

Scott Shaobing Chen, David L Donoho, and Michael A Saunders. Atomic decomposition by basis pursuit. *SIAM review*, 43(1):129–159, 2001.

Rong-En Fan, Kai-Wei Chang, Cho-Jui Hsieh, Xiang-Rui Wang, and Chih-Jen Lin. LIBLINEAR: A library for large linear classification. *Journal of Machine Learning Research*, 9:1871–1874, 2008.

Komei Fukuda, Thomas M Liebling, and Francois Margot. Analysis of backtrack algorithms for listing all vertices and all faces of a convex polyhedron. *Computational Geometry*, 8(1):1–12, 1997.

Peter M Gruber. Aspects of approximation of convex bodies. In *Handbook of Convex Geometry, Part A*, pages 319–345. Elsevier, 1993.

Isabelle Guyon and André Elisseeff. An introduction to variable and feature selection. *Journal of Machine Learning Research*, 3(Mar):1157–1182, 2003.

Satoshi Hara and Masakazu Ishihata. Approximate and exact enumeration of rule models. In *Proceedings of the 32nd AAAI Conference on Artificial Intelligence*, pages 3157–3164, 2018.

Satoshi Hara and Takanori Maehara. Enumerate lasso solutions for feature selection. In *Proceedings of the 31st AAAI Conference on Artificial Intelligence*, pages 1985–1991, 2017.

Stefan König. Computational aspects of the hausdorff distance in unbounded dimension. *arXiv preprint arXiv:1401.1434*, 2014.
Alex Kulesza, Ben Taskar, et al. Determinantal point processes for machine learning. *Foundations and Trends® in Machine Learning*, 5(2–3):123–286, 2012.

Su-In Lee, Honglak Lee, Pieter Abbeel, and Andrew Y. Ng. Efficient l1 regularized logistic regression. In *Proceedings of the 21st National Conference on Artificial Intelligence*, pages 1–9, 2006.

Michel Minoux. Accelerated greedy algorithms for maximizing submodular set functions. In *Optimization Techniques*, pages 234–243. Springer, 1978.

Yannis Pantazis, Vincenzo Lagani, and Ioannis Tsamardinos. Enumerating multiple equivalent lasso solutions. *arXiv preprint arXiv:1710.04995*, 2017.

Ryan J Tibshirani et al. The lasso problem and uniqueness. *Electronic Journal of Statistics*, 7:1456–1490, 2013.

Robert Tibshirani. Regression shrinkage and selection via the lasso. *Journal of the Royal Statistical Society. Series B (Methodological)*, pages 267–288, 1996.

Hui Zou and Trevor Hastie. Regularization and variable selection via the elastic net. *Journal of the Royal Statistical Society: Series B (Statistical Methodology)*, 67(2):301–320, 2005.