Data Twinning
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Abstract
In this work, we develop a method named Twinning, for partitioning a dataset into statistically similar twin sets. Twinning is based on SPlit, a recently proposed model-independent method for optimally splitting a dataset into training and testing sets. Twinning is orders of magnitude faster than the SPlit algorithm, which makes it applicable to Big Data problems such as data compression. Twinning can also be used for generating multiple splits of a given dataset to aid divide-and-conquer procedures and k-fold cross validation.

Keywords: Data compression, Data splitting, Testing, Training, Validation.

1 Introduction

Often in statistics and machine learning we are required to partition a dataset, e.g., when (i) splitting a dataset for training and testing, (ii) subsampling from Big Data for conducting tractable statistical analysis or to save storage space, (iii) generating multiple splits of a dataset for divide-and-conquer procedures to act upon, and (iv) creating k-fold cross validation sets for model tuning and validation. For this purpose, we propose a novel method named Twinning that can be used for partitioning a dataset into statistically similar sets.

Twinning is motivated from the recent work on optimal data splitting for model validation, by Joseph and Vakayil (2021). For model validation, the common practice is to randomly split the dataset into training and testing sets, e.g., for an 80-20 split, 20% of the dataset is selected randomly for testing, while the remaining 80% is used for training the model. It is easy to see that such random splitting can plausibly give rise to pathological splits, wherein the training and testing sets cover roughly disjoint regions of the feature space, thereby resulting in poor testing performance of the model. Clearly there is a need to
systematically split data such that the training set provides sufficient coverage of the feature space. **CADEX** by [Kennard and Stone (1969)](https://www.jstor.org/stable/2337399) marks the beginning of such data splitting procedures in the literature. **CADEX** pushes majority of the extreme points in the feature space into the training set, while in **DUPLEX**, a procedure later presented by [Snee (1977)](https://onlinelibrary.wiley.com/doi/abs/10.1002/9780470316893.ch14) as an improvement over **CADEX**, the extreme points are about equally distributed between the training and testing sets, thereby producing a more robust testing set for validation. [Reitermanova (2010)](https://onlinelibrary.wiley.com/doi/abs/10.1002/9780470316893.ch14) provides a detailed survey of various data splitting procedures that are geared towards this goal.

[Joseph and Vakayil (2021)](https://onlinelibrary.wiley.com/doi/abs/10.1002/9780470316893.ch14) claim that if rows of a given dataset, including the response, are assumed to be independent realizations from a distribution $F$, then an unbiased estimate of the model’s generalization error is obtained when the testing set itself is a realization of $F$. Random data splitting achieves this distributional similarity, but not **CADEX** and **DUPLEX**; furthermore, **CADEX** and **DUPLEX** do not include the response in their computations. The **SPXY** procedure proposed by [Galvao et al. (2005)](https://onlinelibrary.wiley.com/doi/abs/10.1002/9780470316893.ch14) is similar to **CADEX**, but includes the response, even still, the distributional similarity is lacking.

The procedure **SPXY** developed by [Joseph and Vakayil (2021)](https://onlinelibrary.wiley.com/doi/abs/10.1002/9780470316893.ch14) produces testing sets statistically similar to the original dataset. Both parametric and non-parametric models built using **SPXY** exhibit promising results over random data splitting, i.e., improved and consistent testing performance; only caveat being the computational complexity of making the split. Consider some $d$-dimensional datasets generated by sampling from a multivariate normal with $\mu = [0, \ldots, 0]^\top \in \mathbb{R}^d$ and $\Sigma \in \mathbb{R}^{d \times d}$: $\Sigma_{ij} = 0.5^{|i-j|}, \forall i, j \in \{1, \ldots, d\}$. Figure 1 plots the computation time to make an 80-20 split using 500 iterations of the original algorithm for **SPXY** on a 36-core Intel 3.0 GHz processor, against the size of the dataset. Although the algorithm can be executed in parallel, the quadratic growth suggests a two day wait to split the 16-dimensional dataset if it had a million rows, even with access to 36 cores. Hence, though apt for model validation, the computational complexity of **SPXY** holds it back from being applied to Big Data that are prevalent today in every domain. In this work, we develop an efficient algorithm named **Twinning** that is capable of splitting
Big Data with the same objective as SPlit. As will be shown, the computational efficiency of Twinning, coupled with the statistical properties of the splits generated, broadens its applicability to a wide variety of problems that are inaccessible for SPlit.

![SPlit Computation Times](image)

**Figure 1:** Computation times for making an 80-20 split of $d$-dimensional multivariate normal datasets with $N$ rows, using 500 iterations of the original algorithm for SPlit, on a 36-core processor.

The remainder of this article is organized as follows. Section 2 reviews the theory behind SPlit. Section 3 presents the new Twinning algorithm, and Section 4 provides several computational experiments to assess the performance of Twinning. Section 5 extends Twinning for generating multiple splits of the dataset. Section 6 discusses applications of Twinning in data splitting, data compression, and cross-validation. Finally, we state our concluding remarks in Section 7.

## 2 Review of SPlit

Let $\mathcal{D} = \{\mathbf{Z}_i = [\mathbf{X}_i, Y_i]\}_{i=1}^N \in \mathbb{R}^{N \times d}$ be the given dataset, where $\mathbf{X}_i$ is a $d - 1$ dimensional vector representing the $d - 1$ features in the $i^{th}$ row, and $Y_i$ denotes the corresponding
response value. Assume that each row of the dataset is independently drawn from a distribution $\mathcal{F}$:

$$(X_i, Y_i) \overset{iid}{\sim} \mathcal{F}, \ i = 1, \ldots, N.$$ 

The aim is to fit a model $g(X; \theta)$ to the data, where $\theta$ is the unknown set of parameters in the model. To protect against overfitting, we will not use the entire data for estimation. Instead, the dataset is split into two sets: testing set ($D^1$) and training set ($D^2$) with sizes $n$ and $N - n$, respectively. Then, $D^2$ will be used for parameter estimation, and $D^1$ will be used for assessing the model performance.

To quantify the model’s performance, define the generalization error as in Hastie et al. (2009, Ch. 7) by

$$\mathcal{E} = E_{X,Y} \{ L(Y, g(X; \hat{\theta})) | D^2 \},$$

where $\hat{\theta}$ is the estimate of $\theta$ obtained from the training set by minimizing a loss $L(Y, g(X; \theta))$. An estimate of the generalization error can be obtained from the testing set as

$$\hat{\mathcal{E}} = \frac{1}{n} \sum_{i=1}^{n} L(Y^1_i, g(X^1_i; \hat{\theta})),$$

where $U_i = (X^1_i, Y^1_i)$ denote the $i^{th}$ sample in $D^1$. The estimate of the generalization error will be unbiased if

$$U_i \sim \mathcal{F}, \ i = 1, \ldots, n.$$

Random sampling is the easiest method to ensure condition (3). However, random sampling gives a high error rate of $O(n^{-1/2})$ for $|\hat{\mathcal{E}} - \mathcal{E}|$. Mak and Joseph (2018) showed that, under some regularity conditions,

$$|\hat{\mathcal{E}} - \mathcal{E}| \leq C \sqrt{\text{ED}},$$

where $C$ is a constant that does not depend on the testing sample, and $\text{ED}$ is the energy distance (Székely and Rizzo, 2013) between the testing sample and the distribution $\mathcal{F}$. The
energy distance can be estimated from the data using

$$ED_{n,N} := \frac{2}{nN} \sum_{i=1}^{n} \sum_{j=1}^{N} \|U_i - Z_j\|_2 - \frac{1}{n^2} \sum_{i=1}^{n} \sum_{j=1}^{n} \|U_i - U_j\|_2 - \frac{1}{N^2} \sum_{i=1}^{N} \sum_{j=1}^{N} \|Z_i - Z_j\|_2,$$

where $\| \cdot \|_2$ is the $\ell_2$ norm. Since the energy distance does not depend on the model $g(\cdot; \theta)$ nor the loss function $L(\cdot, \cdot)$, a model-independent testing set can be obtained by minimizing the energy distance. The minimizer of the energy distance is referred to as support points [Mak and Joseph, 2018]:

$$\{z^*_i\}_{i=1}^{n} = \arg \min_{\{z_i\}_{i=1}^{n}} \frac{2}{n} \sum_{i=1}^{n} E\|z_i - Z\|_2 - \frac{1}{n} \sum_{i=1}^{n} \sum_{j=1}^{n} \|z_i - z_j\|_2. \quad (5)$$

[Mak and Joseph] (2018) also showed that the error rate of $|\hat{E} - E|$ can be reduced to almost $O(n^{-1})$ by using support points.

Thus, support points computed from (5) could be used as the testing set, which can work much better than a random sample. This is the idea behind SPli(t) (Support Points-based split). However, there is one issue. The solution to (5) need not be a subsample of the original dataset, because the optimization is done on a continuous space. What we really need to do is to solve the following discrete optimization problem:

$$\{U^*_i\}_{i=1}^{n} = \arg \min_{\{z_i\}_{i=1}^{n} \in \mathcal{D}} \frac{2}{n} \sum_{i=1}^{n} E\|z_i - Z\|_2 - \frac{1}{n} \sum_{i=1}^{n} \sum_{j=1}^{n} \|z_i - z_j\|_2. \quad (6)$$

Instead of solving (6) directly, [Joseph and Vakayil] (2021) proposed to solve it in two steps: first solve the continuous optimization in (5) using the difference-of-convex (DC) programming technique [Mak and Joseph] (2018) to obtain an approximate solution to support points, and then use a sequential nearest neighbor assignment to find the closest points in the dataset to the support points. From here on in, we will refer to this two-step approach as DC-NN,
i.e., difference-of-convex programming followed by nearest neighbor assignment. Although much faster than an integer programming solution to (6), the computational complexity of this approach is still high.

To arrive at the computational complexity of the DC-NN algorithm, we begin with the DC program that has a complexity of \( O(dn(n + N)/P) \) per iteration, where \( P \) is the number of processor cores available. Let \( \gamma = n/N \). Then, for \( \tau \) iterations, we obtain

\[
O(\tau dn(n + N)) = O(\tau d\gamma N(\gamma N + N)/P) \\
= O(\tau d\gamma(\gamma + 1)N^2/P) \\
= O(\tau d\gamma N^2/P) : : \gamma \in (0, 1).
\] (7)

The sequential nearest neighbor assignment can be efficiently performed using a \textbf{kd-tree}. Building the \textbf{kd-tree} is \( O(dN \log N) \), and \( n \) nearest neighbor queries are needed, each with worst case complexity \( O(N^{1-\frac{1}{d}}) \) and average case complexity \( O(\log N) \). Thus, the average case complexity of the overall procedure can be expressed as

\[
O(dN \log N + n \log N + \tau d\gamma N^2/P) = O(dN \log N + \gamma N \log N + \tau d\gamma N^2/P) \\
= O((\gamma + d)N \log N + \tau d\gamma N^2/P) \\
= O(dN \log N + \tau d\gamma N^2/P) : : \gamma < 1.
\] (8)

The quadratic growth in complexity, with respect to the size of the dataset, is the major computational bottleneck of \textbf{SP1it}. \cite{Mak2018} also provide a version of the \textbf{DC} program that uses stochastic majorization-minimization, where the expectations in \( E_Dn,N \) are computed based on a random sample from \( D \) within each iteration of \textbf{DC}, instead of using the full dataset. Let us denote this procedure as \textbf{SDC}, wherein a random sample of size \( \min(\kappa n, N) \) is sampled from \( D \) in every iteration. Thus, for the case of \( \gamma < 1/\kappa \), the complexity of \textbf{SDC} for \( \tau \) iterations reduces to \( O(dn(n + \kappa n)/P) = O(\tau d\kappa \gamma^2 N^2/P) \),
and the average case complexity of SDC-NN becomes $O(dN \log N + \tau d\kappa \gamma^2 N^2/P)$, which is an improvement over DC-NN for small values of $\gamma$. However, for large values of $\gamma$, faster algorithms are needed, which leads us to the main topic of this article that is discussed in the next section.

3 Twinning

The aim of Twinning is to partition a dataset into two disjoint sets such that they have similar statistical properties. We will call the two sets as twins. The twins needn’t be of the same size, but they should have similar statistical distributions. Let $D_1 = \{U_i\}_{i=1}^n$ and $D_2 = \{V_j\}_{j=1}^{N-n}$ be the twins such that $D_1 \cap D_2 = \emptyset$ and $D_1 \cup D_2 = D$. Let $ED_{n,N-n}$ be the energy distance between $D_1$ and $D_2$, which is given by

$$ED_{n,N-n} = \frac{2}{n(N-n)} \sum_{i=1}^n \sum_{j=1}^{N-n} ||U_i - V_j||_2 - \frac{1}{n^2} \sum_{i=1}^n \sum_{j=1}^n ||U_i - U_j||_2 - \frac{1}{(N-n)^2} \sum_{i=1}^n \sum_{j=1}^{N-n} ||V_i - V_j||_2.$$

The twins are obtained by minimizing $ED_{n,N-n}$ with respect to $D_1$ and $D_2$, i.e.,

$$\{U_i^*\}_{i=1}^n, \{V_j^*\}_{j=1}^{N-n} = \arg \min_{\{U_i\}_{i=1}^n, \{V_j\}_{j=1}^{N-n}} ED_{n,N-n}$$

subject to: $\{U_i\}_{i=1}^n \cap \{V_j\}_{j=1}^{N-n} = \emptyset$

$$\{U_i\}_{i=1}^n \cup \{V_j\}_{j=1}^{N-n} = D.$$

At first sight, Twinning appears to be a much harder problem than SPlit since we need to perform the optimization in $Nd$ variables instead of $nd$ variables. Interestingly, the following result shows that the objectives of Twinning and SPlit are equivalent.

Proposition 1. Given $n = \gamma N$, $ED_{n,N} = (1 - \gamma)^2 \cdot ED_{n,N-n}$

All the proofs are given in the Appendix. Proposition 1 shows that minimizing the energy distance between $D_1$ and $D_2$ is the same as minimizing the energy distance between $D_1$ and $D$. Thus, to solve (9), we can solve (6) and set $\{V^*\}_{j=1}^{N-n} = D \backslash \{U^*\}_{i=1}^n$. However, as formally stated below, this is a difficult optimization problem.
Proposition 2. The optimization in (6) is $NP$-hard.

Hence, from Propositions 1 and 2, we have that solving (9) to optimality is intractable. An efficient algorithm to obtain a reasonable solution to (9) is presented next.

3.1 Algorithm

There are three parts to $\mathbf{ED}_{n,N-n}$ that we will examine individually, they are

$$
\mathbf{ED}_{n,N-n}^1 := \frac{2}{n(N-n)} \sum_{i=1}^{n} \sum_{j=1}^{N-n} \|U_i - V_j\|_2,
$$

$$
\mathbf{ED}_{n,N-n}^2 := -\frac{1}{n^2} \sum_{i=1}^{n} \sum_{j=1}^{n} \|U_i - U_j\|_2, \quad \text{and}
$$

$$
\mathbf{ED}_{n,N-n}^3 := -\frac{1}{(N-n)^2} \sum_{i=1}^{n} \sum_{j=1}^{N-n} \|V_i - V_j\|_2.
$$

Minimizing $\mathbf{ED}_{n,N-n}^1$ translates to bringing $D^1$ and $D^2$ closer to each other, whereas minimizing $\mathbf{ED}_{n,N-n}^2$ and $\mathbf{ED}_{n,N-n}^3$ causes the points in $D^1$ and $D^2$, respectively, to be spread out. Consider the case of CADEX and SPXY that were alluded to in Section 1, both procedures effectively aim at minimizing $\mathbf{ED}_{n,N-n}^3$ alone, i.e., a well spread out $D^2$ is produced, while nothing can be said about $D^1$ and its statistical similarity to $D^2$. DUPLEX on the other hand focuses on minimizing both $\mathbf{ED}_{n,N-n}^2$ and $\mathbf{ED}_{n,N-n}^3$, still neglecting $\mathbf{ED}_{n,N-n}^1$. DUPLEX is an improvement over CADEX because in essence $D^1$ is now a relatively rigorous validation set as it is more spread out and potentially includes extreme points. When designing the Twinning algorithm, we will incorporate $\mathbf{ED}_{n,N-n}^1$ as well, thereby tying all the three pieces together.

Assume that $\gamma = 1/r$, where $r$ is an integer, i.e., $N = rn$. The dataset $D$ can now be partitioned into $n$ disjoint subsets each with $r$ points in it. At this stage, if a single point is selected from each of the $n$ subsets into $D^1$ and the remaining $r-1$ points into $D^2$, the desired splitting ratio $\gamma$ is achieved. What remains now is to perform the said partitioning.
and the selection within the $n$ resulting subsets in a manner that respects the $\mathbb{E}D_{n,N-n}$
criterion. With this partitioning in mind, we propose a sequential approach where given a
starting position $u_1 \in \mathcal{D}$, the $r - 1$ closest points to $u_1$ in $\mathcal{D}$ together with $u_1$ form the first
of the $n$ subsets. Let this first subset be $S_1 = \{u_1, v_1^1, \ldots, v_r^{r-1}\} \in \mathcal{D}$, here $u_1$ is pushed
into $\mathcal{D}^1$ and the remaining $v_1^1, \ldots, v_r^{r-1}$ are pushed into $\mathcal{D}^2$. For the sake of demonstration,
consider a simple two-dimensional dataset with $\mathcal{N} = 50$ observations generated as follows:
$X_i \sim \mathcal{N}(0, 1)$ and $Y_i | X_i \sim \mathcal{N}(X_i^2, 1)$ for $i = 1, \ldots, N$. We have that $r = 5$ for an 80-20 split.
Plot (a) in Figure 2 depicts the first subset $S_1$, given that we start from the encircled point
labelled as ‘1’ which represents $u_1$.

Next, we select $u_2 \in \mathcal{D} \setminus S_1$ based on some selection rule, and then proceed to identify the
$r - 1$ closest points to $u_2$ in $\mathcal{D} \setminus S_1$. Let $S_1 = \{u_1, v_1^1, \ldots, v_r^{r-1}\}$ be such that $\|u_1 - v_k^{k-1}\|_2 \leq \|u_1 - v_1^1\|_2, \forall k = 2, \ldots, r - 1$, i.e., $v_1^1$ is the closest neighbor to $u_1$ in $S_1$, while $v_r^{r-1}$ is the
farthest. Here we propose a selection rule where we select the closest point to $v_r^{r-1}$ in $\mathcal{D} \setminus S_1$ as $u_2$. Similar to the first subset, let the second subset be $S_2 = \{u_2, v_2^1, \ldots, v_r^{r-1}\} \in \mathcal{D} \setminus S_1$ where $u_2$ is pushed into $\mathcal{D}^1$ and the remaining $v_2^1, \ldots, v_r^{r-1}$ are pushed into $\mathcal{D}^2$. Plot (b) in Figure 2 shows both subsets $S_1$ and $S_2$ where the encircled point labelled as ‘2’ is $u_2$. Now we see the pattern where given $S_{i-1}$, we select the closest point to $v_r^{r-1}$ in $\mathcal{D} \setminus \bigcup_{j=1}^{i-1} S_j$ to be $u_i$. It can happen that when $\gamma$ is restricted such that $1/\gamma$ is an integer, $n \neq \gamma \mathcal{N}$. In such
scenarios, it is straightforward to set $n \leftarrow \lceil \gamma \mathcal{N} \rceil$, which results in the cardinality of the final
subset to be strictly lower than $r = 1/\gamma$, i.e., $|S_n| < r$. Algorithm 1 formally states the
Twinning algorithm. Since the sample dataset has 50 points, for an 80-20 split, we need to
identify 10 subsets: $S_1, \ldots, S_{10}$ each with 5 points in it as described. Figure 2 depicts the
subsets identified at the end of iterations 1, 2, 5, and 10 of Twinning. In plot (d) of Figure 2 the encircled points make up $\mathcal{D}^1$, and the remaining points form $\mathcal{D}^2$.

Twinning attempts to minimize all three parts of $\mathbb{E}D_{n,N-n}$ that are outlined in (10). It is immediately seen that, when the $r$ points in each of the $n$ subsets are closer to each other, we end up reducing $\mathbb{E}D_{n,N-n}$ since for most testing points there are at least $r - 1$ of its neighbors in $\mathcal{D}^2$. In other words, for most testing points there will not be another testing
point closer than its \((r - 1)^{th}\) neighbor, which in turn brings down \(\mathbb{ED}^2_{n,N-n}\). Reduction in \(\mathbb{ED}^3_{n,N-n}\) is given if \(D^2\) is well spread out rather than aggregated in a region. With the proposed selection rule, Twinning sequentially finds subsets \(S_i, \forall i = 1, \ldots, n\) such that most subsets are expected to be adjacent to their previous subset with minimal overlaps. This in turn ensures that \(D^2\), which constitutes all but one point from each subset, sufficiently covers the region of the dataset, thereby reducing \(\mathbb{ED}^3_{n,N-n}\) as alluded.

Algorithm 1 Twinning

1: Input \(D \in \mathbb{R}^{N \times d}\), splitting ratio \(\gamma : 1/\gamma \in \mathbb{Z}\), and starting position \(u_1\)
2: Standardize the columns of \(D\)
3: \(n \leftarrow \lceil \gamma N \rceil\); \(r \leftarrow 1/\gamma\); \(D^1 \leftarrow \{\}\); \(D^2 \leftarrow \{\}\)
4: for \(i \in \{1, \ldots, n\}\) do
5: if \(i \neq 1\) then
6: \(u_i = \arg \min_{u \in D} \{\|u - v_{i-1}^{r-1}\|_2\}\)
7: end if
8: if \(i = n\) then
9: \(r \leftarrow |D|\)
10: end if
11: \(\{v_1^i, \ldots, v_{r-1}^i\} = \arg \min_{\{v^1, \ldots, v^{r-1}\} \in D \setminus \{u_i\}} \{\sum_{j=1}^{r-1} \|v_j - u_i\|_2\}\)
12: \(D^1 \leftarrow D^1 \cup \{u_i\}\); \(D^2 \leftarrow D^2 \cup \{v_1^i, \ldots, v_{r-1}^i\}\); \(D \leftarrow D \setminus \{u_i, v_1^i, \ldots, v_{r-1}^i\}\)
13: end for
14: return \(D^1, D^2\)

Figure 3 shows a pathological random 80-20 split, a split from 500 iterations of DC-NN, as well as the split obtained by Twinning on the same sample dataset. When comparing different splits of a fixed dataset, it is easier to use \(\mathbb{ED}_{n,N}\) as the metric, i.e., energy distance between the smaller twin \(D^1\) and the whole dataset \(D\). Similar to how \(\mathbb{ED}_{n,N-n}\) in [10] has three parts, \(\mathbb{ED}_{n,N}\) also has three parts, of which the third remains constant if the dataset is fixed. Hence, for the remainder of this article, the energy that is being referred to in the plots is

\[\mathbb{ED}^{1,2}_{n,N} := \frac{2}{nN} \sum_{i=1}^{n} \sum_{j=1}^{N} \|U_i - Z_j\|_2 - \frac{1}{n^2} \sum_{i=1}^{n} \sum_{j=1}^{n} \|U_i - U_j\|_2,\]  

(11)
Figure 2: The convex hull of subsets identified by Twinning at the end of iterations 1, 2, 5, and 10 for the sample dataset described in Section 3. Points in $D^1$ are shown as encircled points, and they are numbered in the order they were selected.
where \( \{ Z_i \}_{i=1}^N \) is the dataset and \( \{ U_i \}_{i=1}^n \) is the testing set as before. \( \mathbb{E}D_{n,N}^{1,2} \) for the split obtained from Twinning in Figure 2 is 1.724636. We see that the performance of Twinning comes close to that of DC-NN. In Section 4 we provide an extensive comparison between Twinning and DC-NN, where we find that in higher dimensions and for larger values of \( N \), Twinning edges out DC-NN with substantially lower computation time.

### 3.2 Computational Complexity

Much of Twinning’s computational complexity can be attributed to nearest neighbor queries. Exact nearest neighbor queries in higher dimensions may not be efficient, and several approximate nearest neighbor search algorithms have been proposed in the literature to address this, e.g., locality-sensitive hashing \cite{slaney2008}. Li et al. \cite{li2019} provides a comprehensive evaluation of nineteen such algorithms. Nevertheless, following the implementation of DC-NN \cite{vakayil2021} that uses a \texttt{kd-tree} based exact nearest neighbor search \cite{blanco2014}, we use the same in our analysis of Twinning.

Building the \texttt{kd-tree} is \( \mathcal{O}(dN \log N) \). In each of the \( n \) iterations, Twinning makes one nearest neighbor query to locate \( u_i, i \neq 1 \), and one \texttt{r-nearest neighbors} query to identify
\{v_1^i, \ldots, v_{r-1}^i\}$; the former has a worst case complexity of $O(N^{1-\frac{1}{d}})$, and $O(N^{1-\frac{1}{d}} + r)$ for the latter. The complexity of these nearest neighbor(s) queries is lower in practice, with the average case complexity being $O(\log N)$ \cite{friedman1977}. Updating the \texttt{kd-tree} after each query is an expensive affair, hence, instead of deleting a point after it has been queried out of the tree, the point is merely masked. The overall complexity of \texttt{Twinning} in the worst case can be simplified to

$$O(dN \log N + 2n(N^{1-\frac{1}{d}} + r)) = O(dN \log N + 2\gamma N(N^{1-\frac{1}{d}} + \frac{1}{\gamma}))$$

$$= O(dN \log N + 2(\gamma N^{2-\frac{1}{d}} + N))$$

$$= O(dN \log N + \gamma N^{2-\frac{1}{d}}),$$

while the average case complexity is

$$O(dN \log N + 2n \log N) = O(dN \log N + 2\gamma N \log N)$$

$$= O((\gamma + d)N \log N)$$

$$= O(dN \log N) \quad \because \gamma < 1,$$

which is much better than the complexity of \texttt{DC-NN} given in \cite{8}.

### 4 Experiments

Consider $d$-dimensional datasets with $N$ rows generated by sampling from a multivariate normal with $\mu = [0, \ldots, 0]^\top \in \mathbb{R}^d$ and $\Sigma \in \mathbb{R}^{d \times d}$: $\Sigma_{ij} = 0.5 |i-j|, \forall i, j \in \{1, \ldots, d\}$. In this section we compare \texttt{DC-NN} and \texttt{Twinning} for splitting these datasets. The performance of the splits is measured in terms of the computation time and the energy distance metric $\mathbb{E}d_{n,N}^{1,2}$ defined in \cite{11}. Plot (a) in Figures 4, 5, and 6 considers smaller datasets, where the experiments are run on a laptop with 6-core Intel 2.6 GHz processor, while plot (b) considers bigger datasets, where the experiments are run on a 36-core Intel 3.0 GHz processor. The
plots show the ratio of $\mathbb{E}D_{1,2}^{n,N}$ obtained from Twinning to that obtained from DC-NN; hence, an energy ratio of less than 1 for a given $N$, $d$, and $\gamma$ indicates that Twinning performed better than DC-NN with respect to the quality of the split.

**Twinning** is deterministic when $u_1$ is fixed, and in this section $u_1$ is chosen to be the point farthest from the centroid of the dataset. With DC-NN, the split can vary over multiple runs of the algorithm owing to its random initialization, hence, for stability, 500 iterations of the iterative algorithm that computes support points is used; the quality of the split improves with every iteration of the iterative algorithm. Moreover, DC-NN can be run in parallel, with the computation time being inversely proportional to the number of parallel threads, whereas Twinning is serial. Still, we see that the computation times for Twinning are significantly lower compared to DC-NN. For example, consider plot (b) of Figure 4, where for $N = 10^5$, $d = 16$, and $\gamma = 0.2$, the computation time for Twinning is better than DC-NN by a factor of 27, even though DC-NN is executed in parallel on 36 cores, i.e., if DC-NN were to be executed on a single core, Twinning would observe an improvement in computation time by a factor of $27 \times 36$ over DC-NN. In addition, the quality of the split obtained by Twinning is better than that obtained from DC-NN.

From Figures 4, 5, and 6 it is evident that Twinning outperforms DC-NN, both in terms of computation time and quality of the split, when it comes to bigger datasets. It is when $N$, $d$, and $\gamma$ are all small, DC-NN produces better quality splits than Twinning. Hence, for partitioning Big Data, Twinning is the algorithm of choice.
(a) $d = 4, \gamma = 0.2$

(b) $d = 16, \gamma = 0.2$

Figure 4: Comparison between DC-NN and Twinning for varying $N$ with fixed $d$ and $\gamma$. 500 iterations are used for DC-NN. The red circles and blue diamonds represent the computation times for DC-NN and Twinning, respectively. The green crosses denote the energy ratio of Twinning to DC-NN.

(a) $N = 5000, \gamma = 0.2$

(b) $N = 1.0 \times 10^5, \gamma = 0.2$

Figure 5: Comparison between DC-NN and Twinning for varying $d$ with fixed $N$ and $\gamma$. 500 iterations are used for DC-NN. The red circles and blue diamonds represent the computation times for DC-NN and Twinning, respectively. The green crosses denote the energy ratio of Twinning to DC-NN.
5 Multiplets

It is often desired to split a dataset into multiple disjoint sets. In keeping with the terminology thus far, if we divide the dataset into three sets with similar statistical properties, we call them *triplets*, four sets as *quadruplets*, and so on. In general, we will call the sets *multiplets*.

There are several applications for multiplets. The well studied $k$-fold cross validation approach proceeds by randomly splitting a dataset into $k$ sets ([Hastie et al., 2009]). Moreover, with the technological advances in parallel computing, divide-and-conquer methods that act upon separate blocks of a dataset are becoming increasingly popular for statistical analysis on Big Data ([Guha et al., 2012]).

When it comes to $k$-fold cross validation, an estimate of the generalization error of a given model is made based on the individual error estimates on the $k$ sets ([Rodriguez et al., 2010]). The reliability of these $k$ separate error estimates are bound to improve when the $k$ sets are themselves distributed similar to the whole dataset, as shown by Joseph and
Vakayil (2021). The divide-and-conquer methods split Big Data into, say, \( k \) manageable sets that are analyzed separately and the results are carefully merged to form a combined inference on the Big Data, thereby circumventing the storage and computational limits of analyzing Big Data on a single machine. It is only reasonable to assume that when these \( k \) separate sets are distributed similar to their union, i.e., the Big Data, the quality of the overall inference could improve, albeit further research is needed in this regard.

Here we demonstrate how Twinning can be adapted to split a given dataset \( D \in \mathbb{R}^{N \times d} \) into \( k \) multiplets: \( D^1, D^2, \ldots, D^k \) such that \( \bigcup_{i=1}^{k} D^i = D \) and \( D^i \cap D^j = \emptyset, \forall i \neq j \). For ease of presentation, we will explain the methodology to generate multiplets of the same cardinality, i.e., \( |D^i| = N/k, \forall i \). As defined in (11), let \( E_D^{1,2} \) be the energy of \( D^i \) with respect to \( D, \forall i \), and let \( E_D^{1,2(\ast)} := \max \{ E_D^{1,2} : i \in \{1, \ldots, k\} \} \). A lower \( E_D^{1,2(\ast)} \) indicates that all the \( k \) sets \( D^i, \forall i \) are distributed similar to \( D \). We propose the following three strategies to generate multiplets with Twinning:

\[ S^1 \] Run Twinning on \( D \) with \( \gamma = \frac{n}{N} = \frac{1}{k} \) to obtain \( D^1 \) and \( D \setminus D^1 \). Next, run Twinning on \( D \setminus D^1 \) with \( \gamma = 1/(k-1) \) to obtain \( D^2 \) and \( D \setminus \bigcup_{i=1}^{2} D^i \). Repeat until \( D^{k-1} \) and \( D^k \) are obtained.

\[ S^2 \] Repeatedly run Twinning on \( D \) with \( \gamma = 0.5 \) until all the \( k \) sets \( D^1, \ldots, D^k \) are obtained, assuming \( k \) is a power of 2, i.e., \( k = 2^a : a \in \mathbb{Z} \).

\[ S^3 \] Run Twinning on \( D \) with \( \gamma = \frac{1}{k} \). Let \( S_e, \forall e \in \{1, \ldots, n\} \) be the \( n \) mutually exclusive and collectively exhaustive subsets of \( D \) identified by Twinning. Let \( S_e = \{ u_e, v_e^1, \ldots, v_e^{r-1} \}, \forall e \), where \( r = k \). For subset \( S_e, \forall e \) add \( u_e \) to \( D^1 \), \( v_e^1 \) to \( D^2 \), \ldots, and \( v_e^{r-1} \) to \( D^k \), \( \forall e \in \{1, \ldots, n\} \).

Figure 7 provides a simple depiction of the three strategies \( S^1, S^2, \) and \( S^3 \) for generating quadruplets, i.e., \( k = 4 \). We see that both \( S^1 \) and \( S^2 \) require \( k - 1 \) runs of Twinning, while strategy \( S^3 \) gets away with a single run of Twinning on \( D \). To assess the performance of the three strategies, consider a \( d = 16 \) dimensional dataset with \( N = 10000 \) rows.
Figure 7: Pictorial representation of the three proposed strategies to generate quadruplets of the same cardinality with Twinning.

generated by sampling from a multivariate normal with $\mu = [0,\ldots,0]^\top \in \mathbb{R}^d$ and $\Sigma \in \mathbb{R}^{d\times d}: \Sigma_{ij} = 0.5|i-j|, \forall i,j \in \{1,\ldots,d\}$. We generate quadruplets of this dataset such that $n_i = 2500, \forall i \in \{1,2,3,4\}$ using $S_1$, $S_2$, and $S_3$, wherein Twinning starts from a random $u_1$ in every run. We also make a multi-split randomly for comparison. This experiment is then repeated 250 times on the same dataset, and Figure 8 reports the distribution $\mathbb{E}D^{1,2(\ast)}_{n,N}$ over these 250 multi-splits with the four strategies that includes random splitting. It is readily observed that all the three strategies $S_1$, $S_2$, and $S_3$ perform better than randomly splitting the dataset into 4 sets such that $\mathbb{E}D^{1,2(\ast)}_{n,N}$ is minimized. In addition, we see that strategies $S_1$ and $S_2$ perform better than $S_3$, at the computational cost of additional Twinning runs. However, $S_3$ can only produce multiplets of same cardinality, whereas it is straightforward to generalize $S_1$ and $S_2$ for the case of unequal cardinalities by varying the $\gamma$ in the Twinning runs.
Figure 8: Distribution of $\mathbb{E}_{H_{n,N}}^{1,2(*)}$ over 250 multi-splits of the multivariate normal dataset by random splitting, and the three proposed strategies for generating multiplets with Twinning.

6 Applications

In this section, we discuss several applications of Twinning.

6.1 Data Splitting

Consider the problem of predicting taxicab trip duration from the trip characteristics such as total trip distance and proportion of highway. Here, we use the New York City (NYC) taxicab dataset provided as part of the 2017 kaggle competition. In particular, we use the dataset from Benmeida (2017) that contains 2,074,291 observations. We will use eight continuous features for modeling, as done in Joseph and Mak (2021).

Before fitting the model, we will make an 80-20 split of the dataset, i.e., training set will contain 1,659,432 observations and testing set 414,859 observations. If we were to use DC-NN, splitting alone would have taken about one month to finish on our laptop. SDC-NN would also take similar amount of time because it is the same as DC-NN when $\kappa \geq 5$ and $\gamma = 0.2$. Thus, it is impractical to optimally split this big dataset using DC-NN or SDC-NN.
On the other hand, Twinning was able to make the split in just about two minutes! It is clear that without Twinning one would have to be content with random subsampling. Thus, the remarkable speed of Twinning makes optimal data splitting a reality, especially for Big Data problems.

6.2 Data Compression

In the current data-rich age, computational resources are a bottleneck to analyze or store the vast amount data that is being generated across domains. Furthermore, the trend is set to continue into the foreseeable future, given the lackluster growth rate of computational power over the decade, as we await technological breakthroughs (Theis and Wong, 2017). Hence, we resort to data compression methodologies that attempt to reduce the size of Big Data while retaining complete or partial information from the Big Data. There exists a fundamental limit to lossless data compression (Shannon, 1948), i.e., there is a limit to the extent which a given Big Data can be reduced in size such that no information is lost in the process. The trade-off between the reduction in size and the amount of information retained is what characterizes a lossy data compression that allows for further reduction in size at the expense of information loss.

Twinning can be viewed as a lossy data compression methodology, where a statistically similar subsample is obtained from the Big Data after compression. The statistical similarity can be associated with retention of information, i.e., the more statistically similar a given subsample is to the Big Data, the more information is retained. Either of the twin subsamples produced by Twinning can be the subsample in question, that can be used instead of the Big Data for tractable statistical analysis. As we will see, the computational efficiency of Twinning is a major factor that enables its use for data compression.

Since Twinning is based on support points, it can serve as a model-independent data compression methodology, as opposed to the many model-based compression methods in the literature, e.g., information-based optimal subsample (IBOSS) by Wang et al. (2019).
Additionally, unlike support points, Twinning produces a subsample of the original dataset, and thus, it could be viewed as a data reduction technique in addition to data compression. We note that, although Twinning makes use of the response column(s) in the dataset, it still behaves like an unsupervised data reduction technique, which is quite different from supervised methods for data reduction, e.g., supercompress by Joseph and Mak (2021).

To demonstrate the applicability of Twinning for data compression, consider again the NYC taxi trip dataset introduced in Section 6.1. The training and testing sets have 1,659,432 and 414,859 observations, respectively. Suppose we are interested in fitting a random forest regression model using the randomForest package in R (Liaw and Wiener, 2002). Fitting a random forest under the default settings of this package runs into memory allocation issues. Therefore, data compression is a must to train the random forest. Since it is outright impractical to employ DC-NN for the same task, we will compare the performance of Twinning with random subsampling and SDC-NN with $\kappa = 10$. Consider 90% compression, wherein we apply Twinning on the training set with $\gamma = 0.1$. On a laptop with 6-core Intel 2.6 GHz processor, Twinning takes about 40 seconds to reduce the training set, and it takes 24 minutes to train the random forest on the reduced training set that has 165,944 observations. However, SDC-NN would have taken more than 11 days for the same task and therefore, it is impractical to use SDC-NN for data compression.

| $\gamma$ | Reduction Time | Training Time | Total Modeling Time |
|----------|----------------|---------------|---------------------|
|          | Random | SDC-NN | Twinning | Random | SDC-NN | Twinning |
| 0.1      | 0      | 11* days | 40 sec | 24 min | 24 min | 11* days | 24 min |
| 0.05     | 0      | 2\frac{1}{2}* days | 28 sec | 7 min | 7 min | 2\frac{1}{2}* days | 7 min |
| 0.01     | 0      | 153 min | 15 sec | 27 sec | 27 sec | 153 min | 42 sec |
| 0.005    | 0      | 38 min | 14 sec | 11 sec | 11 sec | 38 min | 25 sec |
| 0.001    | 0      | 101 sec | 13 sec | 2 sec | 2 sec | 103 sec | 15 sec |

Table 1: Time taken to reduce the NYC taxi trip training set, and then fitting a random forest regression, on a laptop with 6-core Intel 2.6 GHz processor. Fields marked with an * are estimates.
Figure 9: Distribution of testing RMSE over 50 repetitions of compressing the NYC taxi trip training set with random subsampling, SDC–NN $(\kappa = 10)$, and Twinning, followed by fitting a random forest regression model.

Table 1 lists the total modeling time under the three compression methods: random subsampling, SDC–NN $(\kappa = 10)$, and Twinning, for $\gamma$ values: 0.10, 0.05, 0.01, 0.005, and 0.001. We can see that the performance of Twinning is quite remarkable—it is almost as fast as the random subsampling-based modeling. On the other hand, SDC–NN is clearly not a feasible data compression method when $\gamma$ is large. To compare the testing performance of the fitted models under the three methods, we repeatedly the experiment 50 times for $\gamma \in \{0.005, 0.001\}$. The testing performance is measured in terms of the root-mean-squared prediction error (RMSE) on the testing set that has 414,859 observations. Figure 9 provides the distribution of RMSE over the 50 repetitions, where we see that the testing performance of the random forest models fitted with Twinning edges out those with random subsampling and SDC–NN. It is quite amazing to see that Twinning outperforms SDC–NN not only in computational time, but also in the quality of splits.
6.3 Cross Validation

In this section, we demonstrate how multiplets can be applied to cross validation, as alluded to in Section 5. Consider the airfoil self-noise dataset (Brooks et al., 1989) from the UCI Machine Learning Repository. The dataset was originally developed at NASA after a series of aerodynamic and acoustic experiments on airfoil blade sections. The dataset has 1,503 observations with five continuous features and a continuous response indicating the sound pressure level in decibels. We will fit a regression model on the dataset with LASSO (Tibshirani, 1996), where the regularization parameter $\lambda$ is estimated by $k$-fold cross validation.

Conventionally, the $k$ folds are obtained by randomly partitioning the dataset into $k$ sets of similar size. Here, we analyze the effect of using multiplets, instead of the random partitions as the $k$ folds, e.g., for 4-fold and 8-fold cross validation, we can use quadruplets and octuplets, respectively. The glmnet (Friedman et al., 2010) package in R is used to fit LASSO, where the same sequence of $\lambda$ values is used when comparing the performance with random folds and multiplets. Let $\lambda_{\text{min}}$ be the $\lambda$ corresponding to minimum mean-squared cross validation error (MSCV). Depending upon the $k$ folds supplied to LASSO, the estimated value of $\lambda_{\text{min}}$ can vary. Consider fitting LASSO on the given dataset with 4-fold and 8-fold cross validation, the left panel of Figure 10 depicts the distribution $\lambda_{\text{min}}$ estimated by LASSO, over 500 distinct random folds and multiplets, while the right panel shows the distribution of MSCV at $\lambda_{\text{min}}$. The multiplets used here are generated by Twinning using the $S^2$ strategy.

It is readily observed from Figure 10 that the use of multiplets for cross validation leads to a stable estimate for the regularization parameter, alongside consistent and smaller MSCV, when compared to random folds. Another interesting takeaway is that even the 4-fold cross validation with multiplets performs better than 8-fold cross validation using random folds, which could prove to be a major computational advantage for tuning computationally expensive models using cross-validation. However, more theoretical investigation and
computational experiments are needed to understand this better, which we leave as a topic for future research.

7 Conclusions

Twinning is built upon the earlier work of Split that is aimed at optimally splitting a dataset into training and testing sets. The existing implementation of Split uses difference-of-convex programming to find support points of the dataset, and then the testing set is sampled from the dataset using a sequential nearest neighbor algorithm (the overall procedure is termed as DC-NN in this article). This procedure can be time consuming, and thus, not applicable to even moderately large datasets. On the other hand, Twinning directly minimizes the energy distance between the two twin sets, and is several orders of magnitude faster than DC-NN. This computational breakthrough allows Twinning to solve many problems that couldn’t even be imagined with Split.
We have described multiple potential applications of Twinning besides data splitting, such as data compression and cross-validation, and have demonstrated its performance on a few real datasets. For example, the taxicab dataset containing more than two million data points were split into two sets of 1.66 million and 0.41 million using Twinning in about two minutes on an ordinary desktop computer. This would not have been possible with DC-NN, which would have taken about a month to compute on a similar computer. This computational advantage is crucial for applications such as data splitting and data subsampling. If an optimal procedure for data subsampling takes more time than fitting a computationally expensive statistical model, then it does not make any sense to subsample the data to save model fitting time, one could rather fit the model directly on the full data. The speed at which Twinning can be executed is quite remarkable that it opens the door to a wide variety of problems to which Twinning can be applied, and we expect many more to be discovered in the future.

Appendix

Proof of Proposition 1

We have that

$$
\mathbb{E} D_{n,N} = \frac{2}{nN} \sum_{i=1}^{n} \sum_{j=1}^{N} \| U_i - Z_j \|_2 - \frac{1}{n^2} \sum_{i=1}^{n} \sum_{j=1}^{n} \| U_i - U_j \|_2 - \frac{1}{N^2} \sum_{i=1}^{N} \sum_{j=1}^{N} \| Z_i - Z_j \|_2
$$

$$
= \frac{2}{nN} \sum_{i=1}^{n} \left\{ \sum_{j=1}^{n} \| U_i - U_j \|_2 + \sum_{j=1}^{N-n} \| U_i - V_j \|_2 \right\} - \frac{1}{n^2} \sum_{i=1}^{n} \sum_{j=1}^{n} \| U_i - U_j \|_2
$$

$$
- \frac{1}{N^2} \left\{ \sum_{i=1}^{n} \sum_{j=1}^{n} \| U_i - U_j \|_2 + 2 \sum_{i=1}^{n} \sum_{j=1}^{N-n} \| U_i - V_j \|_2 + \sum_{i=1}^{N-n} \sum_{j=1}^{N-n} \| V_i - V_j \|_2 \right\}
$$

$$
= \frac{2(N-n)}{nN^2} \sum_{i=1}^{n} \sum_{j=1}^{N-n} \| U_i - V_j \|_2 - \frac{(N-n)^2}{n^2 N^2} \sum_{i=1}^{n} \sum_{j=1}^{n} \| U_i - U_j \|_2 - \frac{1}{N^2} \sum_{i=1}^{N-n} \sum_{j=1}^{N-n} \| V_i - V_j \|_2
$$

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\[
\begin{align*}
\frac{(N - n)^2}{N^2} \cdot \left\{ \frac{2}{n(N - n)} \sum_{i=1}^{n} \sum_{j=1}^{N-n} \|U_i - V_j\|_2 - \frac{1}{n^2} \sum_{i=1}^{n} \sum_{j=1}^{n} \|U_i - U_j\|_2 \\
- \frac{1}{(N-n)^2} \sum_{i=1}^{N-n} \sum_{j=1}^{N-n} \|V_i - V_j\|_2 \right\} \\
= \frac{(N - n)^2}{N^2} \cdot \mathbb{E}d_{n,n-n} = (1 - \gamma)^2 \cdot \mathbb{E}d_{n,n-n}.
\end{align*}
\]

\[\square\]

**Proof of Proposition 2**

To see that the optimization in (6) is indeed \(NP\)-hard, consider the special case where \(n = N/2\), so that we get

\[
\{U_i^*\}_{i=1}^{N/2} = \arg\min_{\{U_i\}_{i=1}^{N/2} \in \mathcal{D}} \frac{4}{N^2} \sum_{i=1}^{N/2} \sum_{j=1}^{N/2} \|U_i - Z_j\|_2 - \frac{4}{N^2} \sum_{i=1}^{N/2} \sum_{j=1}^{N/2} \|U_i - U_j\|_2
\]

\[
= \arg\min_{\{U_i\}_{i=1}^{N/2} \in \mathcal{D}} \frac{4}{N^2} \sum_{i=1}^{N/2} \left( \sum_{j=1}^{N/2} \|U_i - U_j\|_2 + \sum_{j=1}^{N/2} \|U_i - V_j\|_2 \right) - \frac{4}{N^2} \sum_{i=1}^{N/2} \sum_{j=1}^{N/2} \|U_i - U_j\|_2
\]

\[
= \arg\min_{\{U_i\}_{i=1}^{N/2} \in \mathcal{D}} \frac{4}{N^2} \sum_{i=1}^{N/2} \sum_{j=1}^{N/2} \|U_i - V_j\|_2,
\]

where \(\{V_j\}_{j=1}^{N/2} = \mathcal{D} \setminus \{U_i\}_{i=1}^{N/2} \). The optimization problem stated in (13) computes an edge-weighted minimum bisection of a complete graph with \(N\) nodes corresponding to the \(N\) data points in \(\mathcal{D}\), and the Euclidean distance (\(\ell_2\) norm) between the nodes as the edge weights. Since graph bisection is known to be \(NP\)-hard for general graphs (Garey et al., 1974), we have that the optimization in (6) is \(NP\)-hard.

\[\square\]

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