



A Distance-Preserving Matrix Sketch

Leland Wilkinson & Hengrui Luo

To cite this article: Leland Wilkinson & Hengrui Luo (2022) A Distance-Preserving Matrix Sketch, *Journal of Computational and Graphical Statistics*, 31:4, 945-959, DOI: [10.1080/10618600.2022.2050246](https://doi.org/10.1080/10618600.2022.2050246)

To link to this article: <https://doi.org/10.1080/10618600.2022.2050246>



[View supplementary material](#)



Published online: 13 May 2022.



[Submit your article to this journal](#)



Article views: 381



[View related articles](#)



[View Crossmark data](#)



Citing articles: 2 [View citing articles](#)



A Distance-Preserving Matrix Sketch

Leland Wilkinson^{a,b} and Hengrui Luo^c

^aH2O.ai, Mountain View, CA; ^bDepartment of Computer Science, University of Illinois at Chicago; ^cLawrence Berkeley National Laboratory, Berkeley, CA

ABSTRACT

Visualizing very large matrices involves many formidable problems. Various popular solutions to these problems involve sampling, clustering, projection, or feature selection to reduce the size and complexity of the original task. An important aspect of these methods is how to preserve relative distances between points in the higher-dimensional space after reducing rows and columns to fit in a lower dimensional space. This aspect is important because conclusions based on faulty visual reasoning can be harmful. Judging dissimilar points as similar or similar points as dissimilar on the basis of a visualization can lead to false conclusions. To ameliorate this bias and to make visualizations of very large datasets feasible, we introduce two new algorithms that, respectively, select a subset of rows and columns of a rectangular matrix. This selection is designed to preserve relative distances as closely as possible. We compare our matrix sketch to more traditional alternatives on a variety of artificial and real datasets. Supplementary materials for this article are available online.

ARTICLE HISTORY

Received September 2020
Accepted February 2022

KEYWORDS

Dimension reduction;
Frobenius coefficient; Matrix
sketching; Visualization

1. Introduction

For a real data matrix X_{np} of size $n \times p$, we assume that rows represent points and columns represent dimensions in a real metric space (\mathbb{R}^p). We might be interested in visually identifying such features as outliers, duplicate points, anomalies, or unusual distributions. When n and p are moderate in size, we can still use simple plots and statistics to explore such features. When these parameters are larger, however, these simple tasks become unwieldy. While it is not uncommon to see machine learning models with $n > 10^9$ and $p > 10^5$, exploratory visualization of datasets smaller than these extremes can be problematic for the following reasons:

- The data won't fit in memory. We can use a columnar distributed database, but this usually fails to deliver the response times users expect in an interactive exploratory environment (Batch and Elmquist 2017)
- Most display algorithms do not scale to problems this size (Keim 2000)
- We cannot send big data “over the wire” in client-server environments where response time is important.
- Sampling tends to conceal outliers and other singular features.
- Plotting many points on display devices (even megapixel or 4K) produces a big opaque spot. We can use kernels, alpha-channel rendering, binning, and other methods to mitigate overlaps, but this impedes brushing and linking gestures.
- Projections often violate metric axioms—points close together in higher-dimensional space may be far apart in lower-dimensional projections. Conversely, points far apart

in higher-dimensional space may be close together in a projection (Luo et al. 2020).

- Thousands of dimensions overwhelm multivariate displays such as parallel coordinates and scatterplot matrices. They run out of display “real estate.”

1.1. Our Contribution

We address these challenges with a pair of algorithms that subset data matrices. We select a subset of rows and columns of X_{np} :

$$X_{np} \mapsto X_{mp} \mapsto X[a, b]_{mk},$$

where $m \ll n$ and $k \ll p$ and a is a row index array of length m and b is a column index array of length k . We restrict our selection of X_{mk} to be approximately *distance-preserving*, where distances between the rows of X_{mk} are linearly related to the distances between the corresponding rows of X_{mp} .

In sketching the rows in X_{np} , we collect points that are relatively close to each other. Our method depends on computing m Euclidean balls of radius r in p -dimensional space. We choose r to be as small as possible when reducing n to a manageable-sized m .

In subsequently sketching columns in X_{mp} , we produce a submatrix of X_{mp} based on k of its columns. We select these k columns such that distances between the m rows in X_{mk} linearly approximate the distances between the m rows in X_{mp} . Our hope is that this new submatrix X_{mk} is substitutable for X_{np} in visual analytic explorations. Although this is a lossy compression, we are able to retain pointers to the rows and columns of X_{np} that

national_rank	quality_of_education	alumniEmployment	quality_of_faculty	publications	influence	citations	patents	score
1	7	9	1	1	1	1	5	100
2	9	17	3	12	4	4	1	91.67
3	17	11	5	4	2	2	15	89.5
1	10	24	4	16	16	11	50	86.17
4	2	29	7	37	22	22	18	85.21
5	8	14	2	53	33	26	101	82.5
2	13	28	9	15	13	19	26	82.34
6	14	31	12	14	6	15	66	79.14
7	23	21	10	13	12	14	5	78.86
8	16	52	6	6	5	3	16	78.55
9	15	26	8	34	20	28	101	73.82
10	21	42	14	22	21	16	10	73.69
11	31	16	24	9	10	8	9	73.64
1	32	19	31	8	19	23	3	69.49
12	34	77	20	11	9	9	7	66.94
1	26	66	11	40	51	44	34	66.69
2	42	38	19	25	36	43	23	65.76
1	4	101	22	101	67	101	29	65.09
13	62	59	23	3	11	6	13	64.05
14	61	101	15	10	8	10	22	63.11
15	1	101	16	101	28	98	101	61.74
2	24	93	13	101	91	101	28	60.76
16	89	75	17	42	24	34	62	60.55
17	101	101	21	19	3	13	33	59.7
18	64	63	33	17	30	21	21	59.66

Figure 1. Matrix of university ratings.

are not in X_{mk} . Consequently, we can employ our sketching algorithm as a preprocessor for interactive applications.

Using these two algorithms allows subsequent analysis of X_{mk} based on a representative subset of its original columns using frequency-weighted statistical models; the weights for each row of X_{mk} are derived from the number of points inside each of the m balls. The algorithms are designed to work separately or together. RowSketcher can be used alone on deep matrices (many rows) and ColSketcher can be used alone on wide matrices (many columns). Both can be used successively on large, approximately square matrices. If both RowSketcher and ColSketcher are used on a given dataset, our convention is to sketch whichever dimension is larger (n or p) first. This approach improves performance.

Figure 1 contains data on world universities from the cwurData.csv dataset at <https://www.kaggle.com/mylesoneill/world-university-rankings>. The table has been anonymized and consists of a subset of the original dataset. The red cells denote values retained by the row and column sketch algorithms, while the white cells are omitted. The figure shows an actual application of a sketching algorithm so that readers can see exactly what it does.

From the construction side, our algorithms have several distinctive aspects. First, they are scalable to larger datasets with moderate growth of complexity. Second, they work on streaming data and are parallelizable, since updating rows and columns involves additive updates of distances.

Third, our algorithms produce axis-parallel results suitable for visualization; it does not create composites of the input columns and retains interpretability of dimensions in the original dataset.

2. Related Work

We first discuss operations on rows (to reduce the number of points n) and then discuss operations on columns (to reduce dimensionality of points p). For general surveys of big data visualization methods, see (Unwin, Theus, and Hofmann 2007; Ali et al. 2016; Peña et al. 2017). For more detail on feature extraction and dimensionality reduction in visual analytics, see (Fekete and Plaisant 2002; Guyon et al. 2006; Krause et al. 2016).

2.1. Reducing Rows

First, we review row-reducing methods that use the original rows in the reduced matrix, including sampling, clustering, and squashing. Second, we introduce row-reducing methods that create new representative rows in the reduced matrix through aggregation.

2.1.1. Sampling

Sampling from the original data matrix is one way of reducing the sample size n , or the number of rows of the data matrix. A

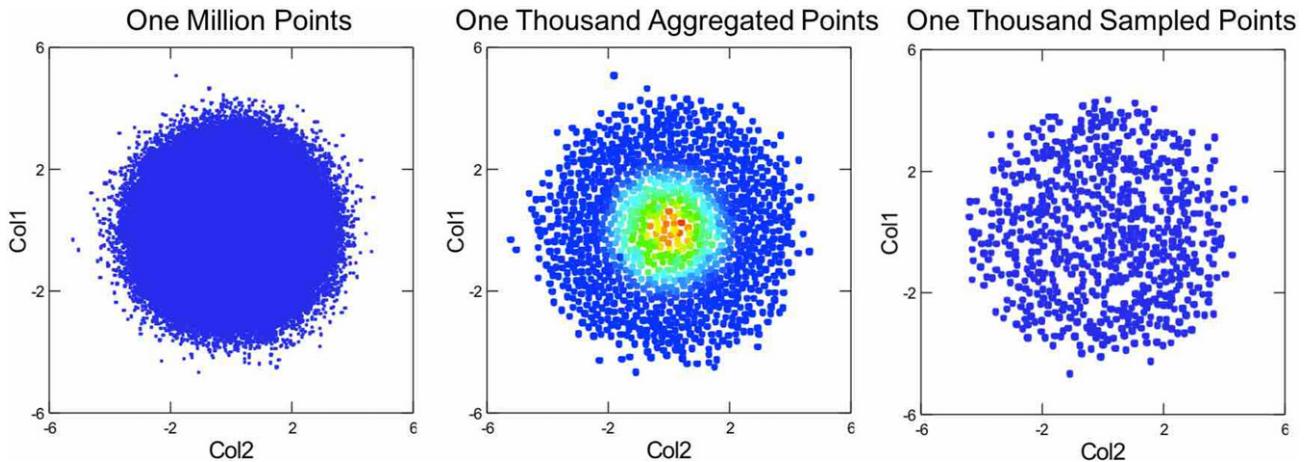


Figure 2. Scatterplots of a million spherical Gaussian (Normal) random numbers (left panel), a thousand aggregated points using the Matrix Row Sketch algorithm (middle panel), and a thousand randomly sampled points (right panel). We have used color to highlight points in the middle panel that have larger frequencies resulting from aggregation. The other two plots contain single points that all have a frequency of 1. We claim that the middle panel scatterplot is a more accurate visual representation of the million-points distribution in the left panel, especially with regard to points at the periphery of the distribution. In addition, the sampled scatterplot in the right panel introduces holes that do not exist in the original or aggregated plot.

well-chosen subsample can represent the original dataset and recover many of the features of the original dataset.

Sampling is not a general solution to our challenges, however. The main problem is that sampling tends to exclude statistical information in areas of low density, especially involving outliers. Unfortunately, these are the features one most wants to see when first exploring a dataset. Figure 2 illustrates this problem. In the rightmost panel of the figure, we see a simple random sample of a million point Gaussian dataset rendered in the leftmost panel. Notice that the outermost points in the raw data plot of a million points do not show up in the sampling plot. The center panel shows our sketching algorithm applied to the same dataset. All the outermost points appear in this plot. And the overall density (a bivariate spherical normal distribution) is more accurately displayed in the central panel.

2.1.2. Clustering

Clustering has been used for decades to reduce a large set of points to a smaller, more tractable, set suitable for subsequent analysis. In this approach, individual points are replaced by their cluster centroids and the count of original points in each cluster is recorded and used in subsequent statistical and visual analytics.

The k -means algorithm is probably the most popular clustering algorithm used for this purpose. It partitions points in a space into k Voronoi cells. In theory, all points in a cell are closer to the centroid of that cell than they are to any other cell centroid. Also in theory, k -means centroids tend to lie in a subspace specified by a principal components decomposition (Park, Jeon, and Rosen 2003; Ding and He 2004a, 2004b).

We qualify these statements with the phrase “in theory” because there are many varieties of k -means algorithms; unfortunately, the theoretical solution is NP Hard (Mahajan, Nimbhorkar, and Varadarajan 2009). Furthermore, identifying the dimensionality of the embedding subspace is not easy. Most k -means algorithms require specifying k in advance of fitting. Ad hoc choices do not guarantee meaningful structure can be identified (Xie et al. 2016). And some measures of cluster-

goodness appear to work well in many cases, but fail in others (Caliński and Harabasz 1974; Rousseeuw 1987)

2.1.3. Squashing

For the purpose of retaining statistical information when n is large, DuMouchel and colleagues coined the term DataSquashing to describe algorithms that attempt to preserve statistical information when “flattening” flat files (DuMouchel et al. 1999). Other similar approaches are reviewed in DuMouchel (2002). These methods work well for certain classes of distributions. They do not claim to be an overall solution to the problem when n is large, however.

2.1.4. Aggregation

An alternative way of reducing the sample size is aggregating. Unlike sampling, aggregating does not necessarily select data points from the original dataset. Instead, it creates new representative data points based on the topology of the original dataset.

One-dimensional Aggregation. The simplest, and probably oldest, form of aggregation involves a single variable. Histogramming is a simple method for aggregating values on a single variable.

1. Choose a small bin width ($k = 500$ bins works well for most display resolutions).
2. Bin rows in one pass through the data.
3. When finished, average the values in each bin to get a single centroid value.
4. Delete empty bins and return centroids and counts in each bin.

An alternative one-dimensional aggregation method is based on dot plots (Wilkinson 1999). Instead of choosing bins of equal width, we stack dots of radius r to represent points. We choose r to result in k stacks; smaller values of r yield more stacks. This algorithm is a one-dimensional version of the row sketching algorithm introduced in this article. *Vector quantiza-*

tion involves dividing a set of points into exclusive subsets. It is equivalent to histogramming with equal or unequal bin widths.

Two-dimensional Aggregation. Two-dimensional aggregation is a simple extension of the one-dimensional histogram algorithm. We take a pair of columns to get (x, y) tuples and then bin them into a $k \times k$ rectangular grid. After binning, we delete empty bins and return centroids based on the averages of the coordinates of members in each grid cell.

Although a little more expensive to compute, *hexagonal bins* (Kosugi et al. 1986; Carr et al. 1987) are preferable to rectangular binning in two dimensions. With square bins, the distance from the bin center to the farthest point on the bin edge is larger than that to the nearest point in the neighboring bin. The square bin shape leads to local anisotropy and creates visible Moiré patterns. Hexagonal binning reduces this effect.

The surface of a sphere is a two-dimensional object. Consequently, we can bin (x, y) tuples on a globe. It seems reasonable to select hexagons to tile the globe, but a complete tiling of the sphere with hexagons is impossible. Compromises are available, however. Carr et al. (1997) and Kimerling et al. (1999) discuss this in more detail.

n -dimensional Aggregation. Unfortunately, high-dimensional aggregation cannot be accomplished through simple extensions of 2D binning. Tiling high-dimensional spaces is problematic (Sayood 2012).

A number of papers attack the high-dimensional problem through 2D slices of the nD data. One of the best applications is also one of the oldest: the Grand Tour (Asimov 1985). A more recent implementation follows a different route through space based on Hamiltonian paths (Hurley and Oldford 2011). Both smoothly animate the path of 2D projections and give users the chance to control the process. But a collection of 2D binnings across an nD space does not accurately reflect or necessarily reveal joint structures in n dimensions. Other subspace aggregations share similar problems. Preaggregated hash tables, for example, can improve response time from databases, but they are useful mainly for low-dimensional tables (Pahins et al. 2016). Other approaches include machine-guided subspace views (Xie et al. 2009; Krause et al. 2016).

2.2. Reducing Columns

In this section, we review column-reducing methods that output the original columns in the reduced matrix. Then we review column-reducing methods that creates new representative columns in the reduced matrix through projections.

2.2.1. Feature Extraction

Feature extraction involves finding a subset of features (columns) that can be used in subsequent analytics or visualizations. Most of these methods involve cluster analysis (in one form or another) or principal components (Cheng, Fu, and Zhang 1999; Dy and Brodley 2004; Friedman and Meulman 2004; Guyon et al. 2006). These two classes of analytics are used to decompose variation in order to identify columns most contributing to that subspace variation.

Unlike projection methods we will introduce below, and like matrix sketching, these approaches aim to produce sets of original variables rather than composites so that interpretation of results can be made in the original data space. However, some feature extraction methods may not depend on statistical procedures like cluster analysis or PCA and sometimes they do not rest on assumptions concerning the distribution of the data.

2.2.2. Projection

A projection, in the restricted sense employed in most visual analytics, is the mapping of a set of points in p dimensions to a subspace of k dimensions. This kind of projection can involve a linear map (as with principal components) or a nonlinear map (as in manifold learning). These methods can also be used for modeling (as in unsupervised learning) or as preliminary steps in feature engineering (Tatu et al. 2011; Cavallo and Demiralp 2018).

Linear Projection. Principal Component Analysis (PCA) is among the most popular linear dimension reduction methods. The original statistical algorithm for computing principal components (Pearson 1901; Hotelling 1933), begins with a covariance matrix S derived from the product of a column-centered X matrix and its transpose and computes an eigendecomposition of that matrix (Equation (1)),

$$S = X^T X / n = V D V^T \quad (1)$$

where the D is a diagonal matrix of eigenvalues and V is a matrix of eigenvectors. The PCA projects the data matrix linearly to the principal component directions.

Principal components were originally designed for multivariate normally distributed points with zero mean. They can still be useful for snapshots of other types of data. More recent methods like nonlinear principal components (Hsieh 2009) and sparse principal components (Zou, Hastie, and Tibshirani 2006) are more flexible.

The Singular Value Decomposition (SVD) works directly on a rectangular matrix. It is a generalization of the Principal Components decomposition, as Equation (2) shows. The SVD algorithm bypasses the need for computing the covariance matrix S .

$$\begin{aligned} X &= UDV^T \\ X^T X &= (UDV^T)^T UDV^T = VD^T U^T UDV^T = VD^2 V^T \end{aligned} \quad (2)$$

Linear projections may not preserve metrics, and therefore, geometry of the dataset (Luo et al. 2020). A major group of existing visualization procedures when p is large make use of dimension reduction via linear projections. However, projections often violate metric axioms—points close together in higher-dimensional space may be far apart in lower-dimensional projections. Conversely, points far apart in higher-dimensional space may be close together in a projection.

Nonlinear Projection. The development of nonmetric multidimensional scaling of symmetric similarity or dissimilarity matrices in the 1960s (Shepard 1962a, 1962b; Kruskal 1964) led to interest in projecting rectangular data into low-dimensional subspaces. Caroll and Chang at Bell Laboratories developed

a topological embedding program called *PARAMAP* (Shepard and Carroll 1966). Since then, numerous researchers have developed models and programs along similar lines (Roweis and Saul 2000; Tenenbaum, de Silva, and Langford 2000; Belkin and Niyogi 2003; van der Maaten and Hinton 2008; McInnes, Healy, and Melville 2018).

These *manifold learning* methods, linear or nonlinear, assume points lie near a k -dimensional manifold embedded in a subspace of the p -dimensional ambient space and they assume the conditional distribution of the distances of points to the manifold (residuals) is random and relatively homogeneous. Unlike principal components, however, manifold learning methods do their best when the distribution of errors is close to a manifold; they do not do well with data containing substantial error.

Nonlinear projections, although attempting to preserve local geometric features, can also violate metric axioms, which can be harmful. For example, a low-dimensional map from a higher-dimensional space that induces viewers to infer that *dissimilar* points in the higher-dimensional space are *similar* can lead to false conclusions. Conversely, a low-dimensional map from a higher-dimensional space that induces viewers to infer that *similar* points in the higher-dimensional space are *dissimilar* can lead to false conclusions. This is a commonly-expressed warning in the manifold learning community (Wattenberg, Viégas, and Johnson 2016).

2.3. Reducing Rows and Columns

Matrix Sketching (Liberty 2013) reduces rows or columns or both simultaneously. Our algorithm is a form of matrix sketching. In general, matrix sketching represents a matrix X through a sketch matrix \tilde{X} such that the error $\|X^T X - \tilde{X}^T \tilde{X}\|$ is relatively small.

2.3.1. CUR Decompositions

We exemplify the matrix sketching method using the CUR decomposition. The CUR decomposition is similar to the Singular Value Decomposition (SVD) (Stewart and Stewart 1998; Drineas, Mahoney, and Muthukrishnan 2008):

$$X = CUR \quad (3)$$

For X_{np} the CUR components are dimensioned as C_{nk} , U_{km} and R_{mp} , where $1 \leq m \leq n$ and $1 \leq k \leq p$. This restriction forces Equation (3) to be an approximation rather than an isometry. Some CUR algorithms are relatively efficient (Drineas, Mahoney, and Muthukrishnan 2008); their time performance can be $O(np^2)$.

The same kind of rank reduction can be achieved with an SVD. Unlike SVDs, however, the matrices C and R are subsets of the rows and columns of X rather than linear combinations of them. This feature of CUR, shared by our matrix sketching algorithm, is distinctive.

However, CUR differs from our algorithm in at least two respects. First, CUR outputs three matrices while ours outputs one. Second, the CUR algorithm leaves n and p unchanged in the C and R matrices. By contrast, our algorithm reduces n and

p to m and k , respectively. For a more general survey of matrix decompositions suited to high-dimensional data, see (Halko, Martinsson, and Tropp 2011).

3. A New Matrix Sketching Algorithm

Our matrix sketch is based on two associated algorithms. We first consider sketching rows to reduce n . Then we consider sketching columns to reduce p .

3.1. Sketching Rows

Our algorithm for reducing the number of rows is related to a greedy approximate solution to the *k-center problem* (Cormode and McGregor 2008):

Given n points in p -dimensional metric space and an integer $k \leq n$, find the minimum radius r and a set of balls of radius r centered on each of m points such that all n points lie within the union of these balls.

Instead of conditioning on k , however, we condition on r and denote the final number of centers to be m in following discussion. Our algorithm is derived from a variant of the Leader clustering algorithm, which is described in Hartigan (1975). **Algorithm 1** shows the rows sketching algorithm.

```

Data:  $X_{n,p}$  (data matrix)
Input:  $r = 0.25/(\log n)^{1/p}$  (default value)
EuclideanDistance ( $a, b$ ) is a Euclidean distance function
Result: exemplars (list of ball centers), members (list of lists)
begin
     $m = 1$ 
    row (array of length  $p$ ) = first row of  $X$ 
    exemplars = new list, initialized to contain row
    members = new list of lists, initialized to contain empty list
    end
    for  $i = 1, \dots, n$  do
        newExemplar = true
        row =  $X[i, .]$  (ith row of  $X$ )
        for  $j = 1, \dots, m$  do
             $d = \text{EuclideanDistance}(\text{row}, \text{exemplars}[j])$ 
            if  $d < r$  then
                add  $i$  to members[ $j$ ]
                newExemplar = false
                break
            end
        end
        if newExemplar then
             $m = m + 1$ 
            add row to exemplars[ $m$ ]
            add new list to members[ $m$ ], initialized with  $i$ 
        end
    end

```

Algorithm 1: RowSketcher Algorithm

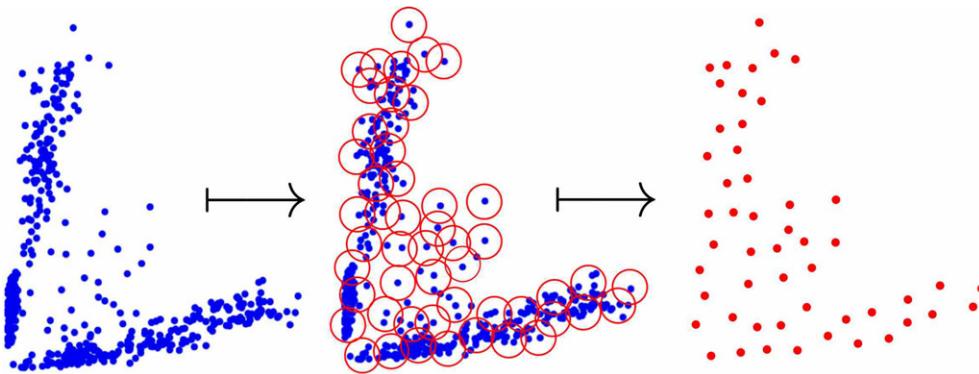


Figure 3. Visualization of the row sketching algorithm in a 2D space.

3.1.1. Notes on RowSketcher Algorithm

1. The default value of r is designed roughly to be below the expected value of the distances between $n(n - 1)/2$ pairs of points distributed randomly in a p dimensional unit hypercube. Increase r to produce fewer exemplars, decrease to produce more.
2. The *exemplars* list contains a list of row values representing points defining exemplar neighborhoods.
3. The *members* list of lists contains one list of indices for each exemplar pointing to members of that exemplar's neighborhood.
4. A consequence of aggregating rows is that statistics on the aggregates must include frequency weighting. This requirement rules out some statistical libraries that do not incorporate frequencies. Most statistical packages for survey analysis, for example, incorporate frequency weighting in their basic statistics (or, in the case of SAS, SPSS, SYSTAT, or STATA, everywhere).
5. The Leader algorithm (Hartigan 1975) creates exemplar-neighborhoods in one pass through the data. It is equivalent to centering balls in p dimensional space on points in the dataset that are considered to be exemplars. Unlike k -means clustering, the Leader algorithm
 - (a) centers balls on actual data points rather than on centroids of clusters,
 - (b) constrains every ball to the same radius rather than allowing clusters to have different diameters,
 - (c) involves only one pass through the data rather than iterating to convergence via multiple passes,
 - (d) produces many balls rather than a few clusters.
6. In rare instances, the resulting exemplars and members can be dependent on the order of the data, but not enough to affect the description of the joint density of points because of the large number of exemplars produced. We are characterizing a high-dimensional density by covering it with many small balls. Even relatively tight clusters produced by a clustering algorithm will be chopped into pieces by the Leader algorithm. Nevertheless, if this is a concern, we can visit the list of exemplars in random order on each iteration.
7. The time complexity of [Algorithm 1](#) is $O(nmp)$.

[Figure 3](#) shows a schematic depicting a 2D implementation of our algorithm.

3.1.2. Categorical Variables

To incorporate categorical variables in the RowSketcher algorithm, we need to convert categories to numerical values. Correspondence Analysis (CA) (Greenacre 1984; Greenacre and Blasius 2006) suits our purpose. We begin by representing a categorical variable with a set of dummy codes, one code (1 or 0) for each category. These codes comprise a matrix of 1's and 0's with as many columns as there are categories for that variable. We then compute a principal components decomposition of the covariance matrix of the dummy codes. This analysis is done separately for each of k categorical variables in a dataset. CA scores on the rows are computed for each categorical variable by multiplying the dummy codes on that row's variable times the eigenvectors of the decomposition for that variable. Computing the decomposition separately for each categorical variable is equivalent to doing a multiple correspondence analysis separately for each variable instead of pooling all the categorical variable dummy codes into one matrix. This application of CA to deal with the visualization of nominal data was first presented in Rosario et al. (2004).

Unfortunately, this approach loses the mapping of rows to specific categories. When members are assigned to exemplars, the category values of the exemplars must be chosen. If we are interested in grouping by category, we must implement a different approach. Namely, we maintain categories in separate cells (e.g., hash table entries) and then apply RowSketcher separately to the continuous values in each cell. If one or more categorical variables have high cardinality, however, this approach has become increasingly impractical.

3.1.3. Performance of RowSketcher Algorithm

[Table 1](#) is based on the million Gaussians dataset used for [Figure 2](#). The three stub panels show the results of computing basic statistics on three different datasets. The Sketch Dataset uses our RowSketcher algorithm (with radius = 0.119) and the Random Sample uses a simple random sample to extract 200 rows from the million. Both row-reducing methods do quite well overall, but there is a striking difference. RowSketcher yields the maxima and minima of the raw dataset, but the Sample method does not. In short, RowSketcher, coupled with frequency-weighted formulas, does quite well on basic statistics.

The first two rows of [Table 2](#) show the results of comparisons between the Row Sketch algorithm and the CUR algorithm. For

Table 1. Original versus row sketch and random sample of a million Gaussians.

	X	Y	Z
Original dataset			
m	1,000,000	1,000,000	1,000,000
n	1,000,000	1,000,000	1,000,000
Min	-4.683	-5.208	-5.184
Max	5.061	4.702	4.832
Mean	-0.001	0.000	0.001
Median	0.000	0.001	0.001
SD	1.000	1.000	1.001
Sketch dataset			
m	200	200	200
n	1,000,000	1,000,000	1,000,000
Min	-4.683	-5.208	-5.184
Max	5.061	4.702	4.832
Mean	0.009	0.001	-0.003
Median	-0.007	0.076	0.031
SD	1.104	1.124	1.127
Random sample			
m	200	200	200
n	1,000,000	1,000,000	1,000,000
Min	-2.916	-2.539	-2.628
Max	2.950	2.513	3.002
Mean	-0.049	-0.020	-0.015
Median	-0.048	0.013	0.010
SD	1.011	0.939	1.046

Table 2. Performance of Sketcher versus CUR algorithm.

	Rows	Cols	rows	cols	CPU	corr	Hit
Outlier2D dataset							
RowSketcher	1000	2	500	2	39 ms	NA	Yes
CUR	1000	2	500	2	53 ms	NA	No
Inlier2D dataset							
RowSketcher	1000	2	500	2	36 ms	NA	Yes
CUR	1000	2	500	2	59 ms	NA	No
Cluster dataset							
ColSketcher	1000	100	1000	2	887 ms	0.99	Yes
CUR	1000	100	1000	2	355 ms	0.82	No
Donut dataset							
ColSketcher	1000	100	1000	2	886 ms	0.96	Yes
CUR	1000	100	1000	2	486 ms	0.68	No
Outlier dataset							
ColSketcher	1000	100	1000	2	899 ms	0.98	Yes
CUR	1000	100	1000	2	360 ms	0.53	No

these comparisons, we coded the Linear Time CUR algorithm (Drineas, Kannan, and Mahoney 2006) in Java and ran the Java versions of our sketching algorithms.

For the Outlier2D test, we generated a thousand bivariate normal points in two dimensions ($\rho = 0.8, \sigma = 0.1$) and added an outlier at (0.6, 0.6). We then asked both algorithms to sketch the dataset down to 500 rows. The RowSketcher algorithm included the outlier, but the CUR algorithm did not.

For the Inlier2D test, we generated a thousand points aligned on a unit circle with a polar conditional Normal standard deviation of 0.1. The resulting scatterplot resembled a donut sprinkled with random Normal points on its surface. In addition, we added one more point at (0, 0) in the center of the donut that we called an “inlier.” As before, we asked both algorithms to sketch the dataset down to 500 rows. The RowSketcher algorithm included the inlier, but the CUR algorithm did not.

For exploratory visualization, any sketching algorithm should capture anomalous points (outliers and inliers) so that

we can analyze them before doing statistical modeling. Because of the distance properties inherent in our Leader algorithm, this is a likely result and desirable property of our row sketching.

3.2. Sketching Columns

Algorithm 2 contains the ColSketcher algorithm.

Data: $X_{m,p}$ (data matrix sketched with [Algorithm 1](#))
Input: $\text{maxCorrelation} = 0.95$ (default value)
 $\text{sum}(a, b)$ is an element-wise sum function on two arrays
 $\text{dist}(X_{m,p})$ produces an $m(m - 1)/2$ array of squared distances
 $\text{FrobeniusCorrelation}(a, b) = (a \cdot b) / (\|a\| \|b\|)$
Result: selectedCols (list of selected columns)
begin
 $\text{correlation} = 0.0$
 $\text{selectedCols} =$ list of selected columns initialized empty
 $\text{previousColDist} = m(m - 1)/2$ length array of zeros
 $\text{allColDist} = m(m - 1)/2$ array of distances from $\text{dist}(X_{.,.})$
end
while $\text{correlation} < \text{maxCorrelation}$ **do**
 $\text{bestColumn} = 0$
 $\text{bestCorrelation} = 0.0$
 $\text{previousBestCorrelation} = 0.0$
 for $j = 1, \dots, p$ **do**
 if $j \notin \text{selectedCols}$ **then**
 $j\text{ColDist} = \text{dist}(X_{[.,j]})$
 $\text{cumColDist} = \text{sum}(j\text{ColDist}, \text{previousColDist})$
 $\text{correlation} =$
 $\text{FrobeniusCorrelation}(\text{cumColDist}, \text{allColDist})$
 if $\text{correlation} > \text{bestCorrelation}$ **then**
 $\text{bestColumn} = j$
 $\text{bestCorrelation} = \text{correlation}$
 end
 end
 end
 $\text{bestColDist} = \text{dist}(X_{[.,\text{bestColumn}]})$
 $\text{previousColDist} = \text{sum}(\text{bestColDist}, \text{previousColDist})$
 add bestColumn to selectedCols
 $\text{previousBestCorrelation} = \text{bestCorrelation}$
end

Algorithm 2: ColSketcher Algorithm

3.2.1. Notes on ColSketcher Algorithm

- Our column sketching algorithm is based on a variant of greedy forward feature selection with a Frobenius coefficient to measure similarity between distance matrices.
- Our algorithm accumulates squared distances in cumColDist on each iteration over p . This saves time by confining distance computations at each step to a pair of column arrays rather than to a matrix of columns. Since squared distances are additive, we need to compute only one-dimensional distances in each step and cumulate them with previously-computed squared distances.
- The time complexity of [Algorithm 2](#) is $O(kmp)$.

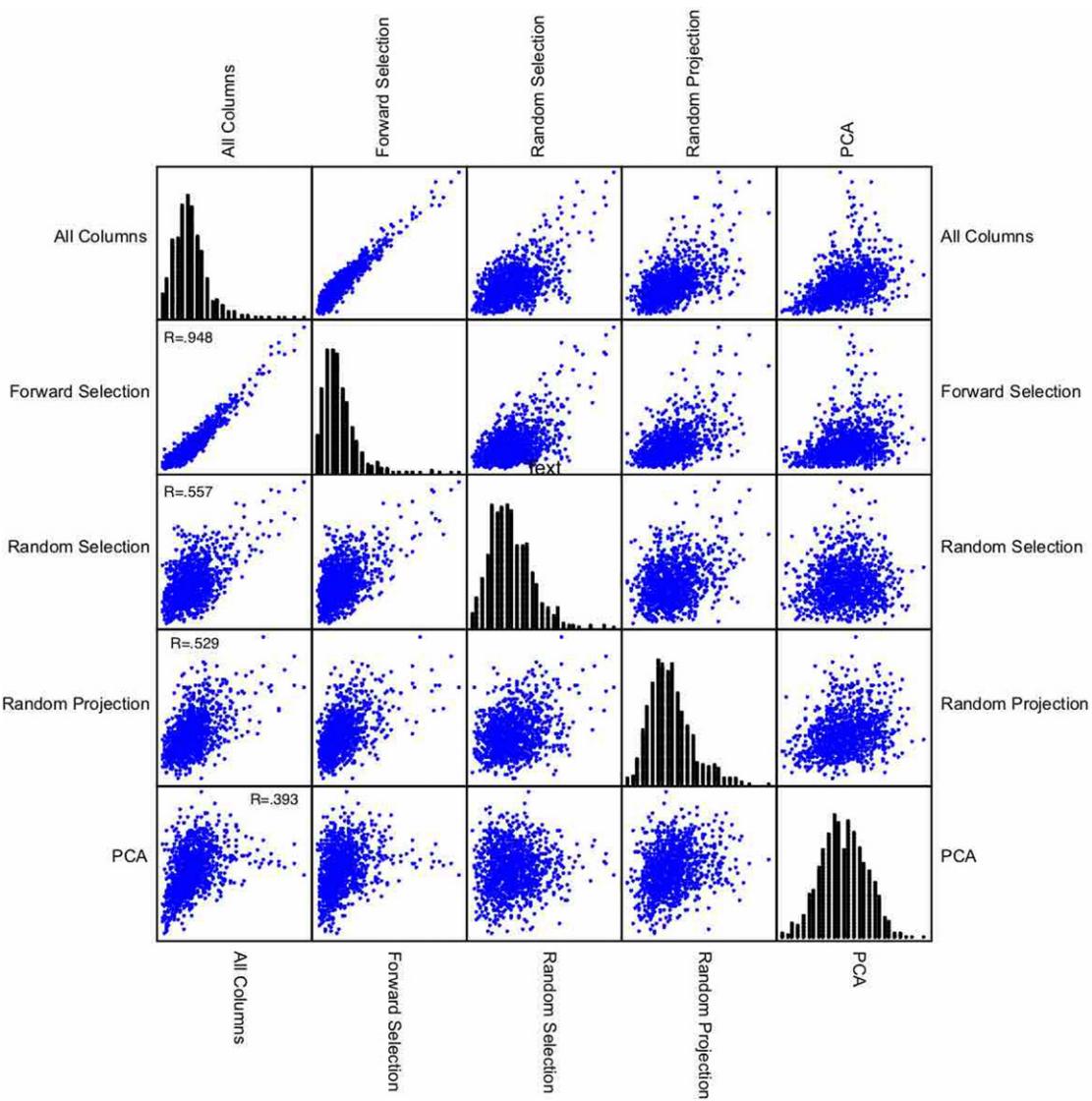


Figure 4. Comparison of column reducing algorithms using the gene expression dataset. The points in the plots represent all pairwise distances between points in higher-dimensional space (20,531 dimensions) and pairwise distances between the same points in projected space (40 dimensions). The forward selection ColSketcher is the only algorithm in this collection that substantially preserves relative distances among points.

3.2.2. Performance of ColSketcher Algorithm

We present in this section various approaches to evaluating the performance of the column sketching algorithm. Some of these are designed to illustrate differences from other algorithms rather than overall effectiveness.

Feature Detection. The last three rows of Table 2 show the results of comparisons between our Column Sketch algorithm and the CUR algorithm. For the Cluster test, we generated a thousand $N(0, 0.1)$ points in 100 dimensions. In two of these dimensions (columns) we randomly centered each of these points on one of six cluster centroids located on a 3×3 grid. We then asked each algorithm to reduce the 100 columns to 2 columns. Our Column Sketcher algorithm correctly located these two columns. The CUR algorithm did not.

For the Donut Dataset test, we generated the same donut we used for the row sketching test, but this time we embedded it in only two of the 100 dimensions. As before, we asked each algorithm to reduce the 100 columns to 2 columns. Our Col-

umn Sketcher algorithm correctly located these two embedding columns. The CUR algorithm did not.

For the Outlier dataset, we generated a thousand bivariate Normal points ($\rho = 0.8, \sigma = 1$), but we embedded them in only two of the 100 dimensions. The remaining columns contained coordinates based on random Gaussians having standard deviations of 0.1. We then added one outlier in the bivariate target columns pair at (6, 6). We then asked each algorithm to reduce the 100 columns to 2 columns. Our Column Sketcher algorithm correctly located these two columns. The CUR algorithm did not.

Distance Preservation. The loss functions and error bounds for many of these projection methods are variously based on the discrepancy between the coordinates of the points in the low-dimensional embedding space and their coordinates in the higher-dimensional residual space. The loss function for *ColSketcher*, by contrast, is based on the correlation between the distances reproduced by the sketch matrix and the original



Figure 5. Comparison of analyses based on the column sketch algorithm (lower panel) and all columns (upper panel) using a cereals dataset from kaggle.

distances between points. In short, most popular projection methods, with the exception of multidimensional scaling, which is challenging to apply on large datasets (Paradis 2018), are not distance-preserving. For details, Cutura et al. (2020) have developed a tool to examine distance preservation visually.

We can compare the distance-preserving capabilities of several column-reducing algorithms. Figure 4 shows a SPLOM of the column sketch algorithm versus several other projection methods. The data are taken from the gene expression dataset used in Figure 9. In all methods, we reduced 20,531 columns to 40 columns. While this reduction might not have been optimal for all methods, it allows us to compare the preservation of distances after the same amount of reduction. The results are dramatic. Clearly, the column sketch outperforms the other methods. Incidentally, we omitted manifold learning methods because they are not distance preserving algorithms; they are

designed to upweight short distances and downweight long ones.

Accuracy of ColSketcher. A simple test of the column sketching algorithm is to compute two analyses of the same data—one on the full dataset and the other on the column-sketched dataset. Figure 5 shows two multidimensional scalings. The upper panel shows the scaling of 77 cereals from a kaggle dataset (<https://www.kaggle.com/crawford/80-cereals>). There are 13 continuous variables represented by the columns (calories, protein, fat, sodium, fiber, carbo, sugars, potassium, vitamins, shelf, weight, cups, rating). We computed Euclidean distances among the cereals based on all 13 columns and then did an MDS on the resulting distance matrix. The cereals are colored blue in this coordinate plot.

The lower panel, in black, shows the scaling of the same cereals using seven columns selected by the column sketch

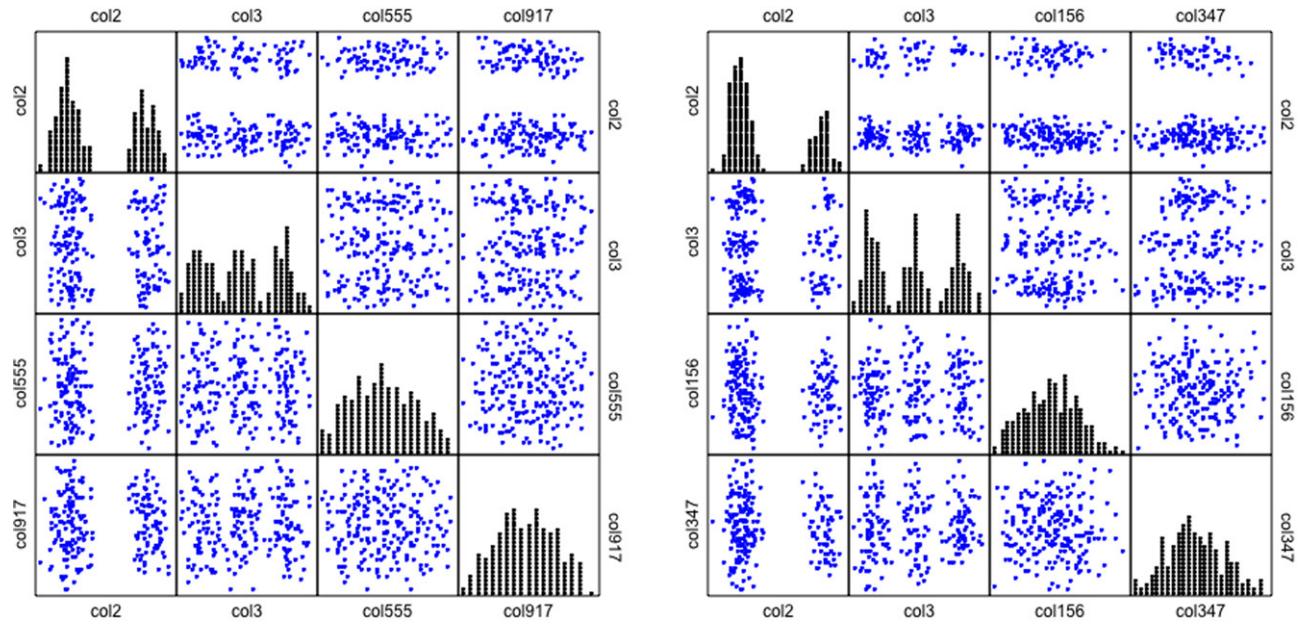


Figure 6. SPLOM on 1000 rows and 1000 Gaussian columns reduced to 4.

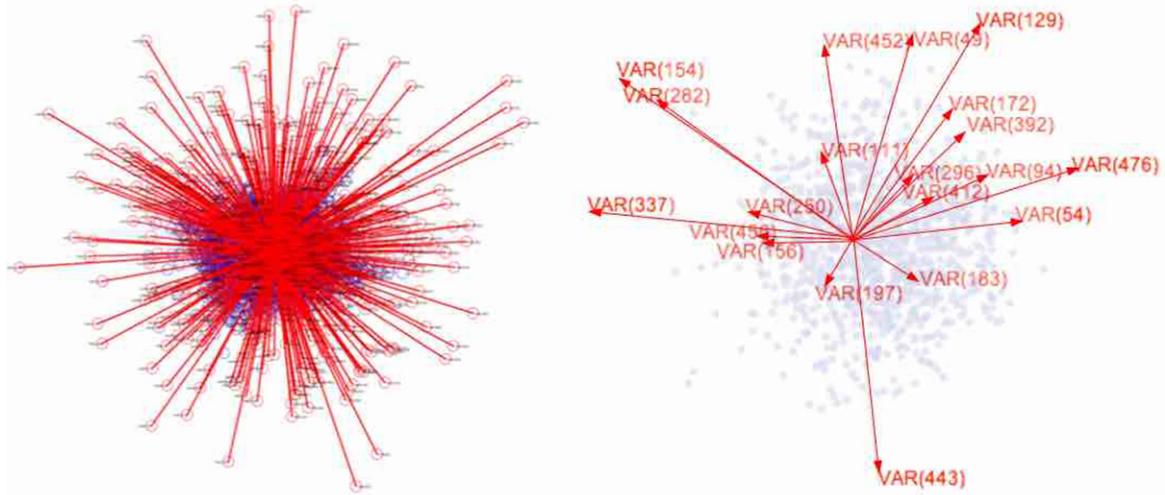


Figure 7. Full Madelon dataset biplot (left) and matrix sketched dataset biplot (right).

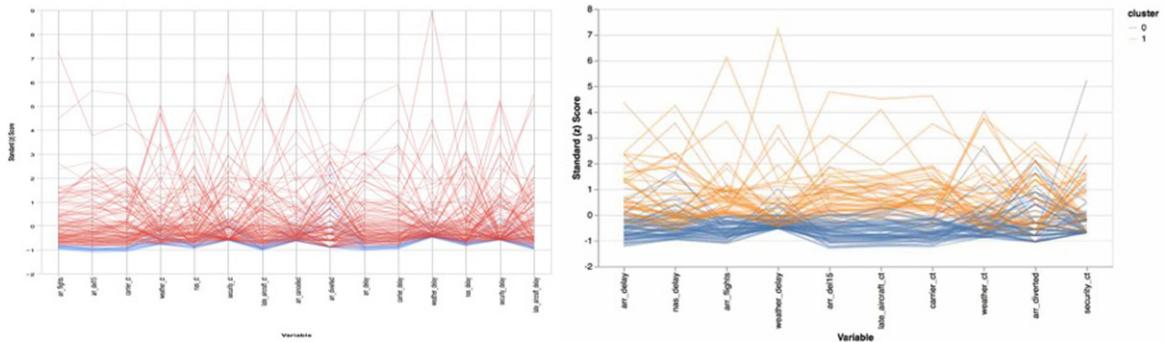


Figure 8. Parallel coordinates plot of 1762 rows reduced to 99 and 15 columns reduced to 10 columns.

algorithm (calories, sodium, fiber, sugars, potassium, vitamins, shelf). The Frobenius correlation between the row distances in the full dataset and in the sketch dataset is 0.98. While there are some differences in detail, the result of the sketch algorithm is

visibly close to the result based on all the variables. This will not be necessarily true if we use analytic visualization methods that do not preserve distances (such as principal components, tSNE, or UMAP).

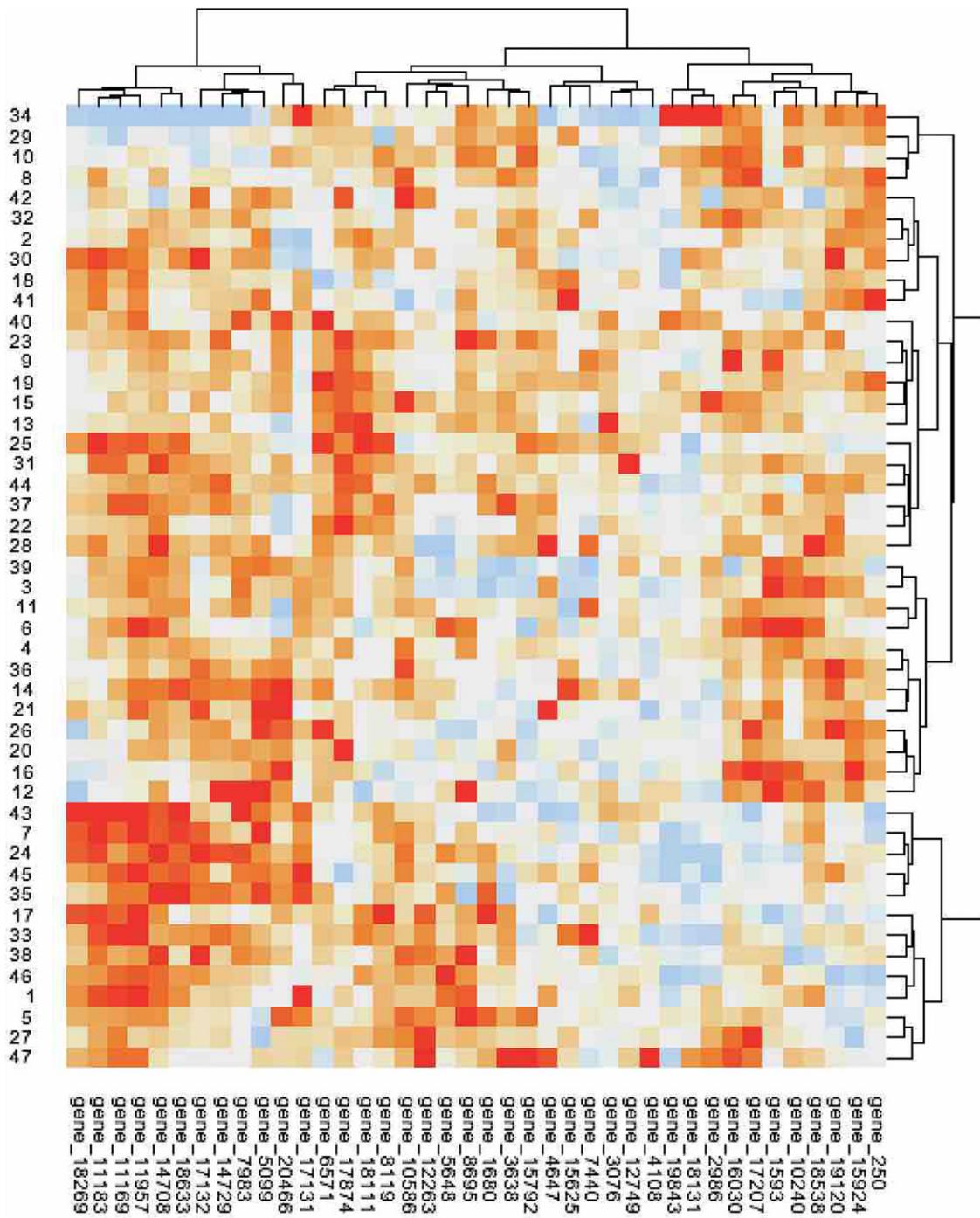


Figure 9. Heatmap of matrix-sketched gene expression data.

Sketching Approximately Square Matrices. Figure 6 shows scatterplot matrices on sketched rows and columns of an artificial dataset. We generated 1000 independent Gaussians on each of 1000 variables. For the third and fourth variables, we generated two and three Gaussians, respectively, separated into clusters. For the left panel, we ran RowSketcher and then ran ColSketcher on the output from RowSketcher. For the right panel, we ran the two sketchers in the opposite order. In both cases, we forced it to select four variables out of the 1000. Figure 6 shows that either sketcher orderings selected the two anomalous variables, col2 and col3. The additional scatterplots show the remaining patterns that are embedded in

this multivariate dataset. Any of the additional variables would have revealed the same patterns when plotted against each other or against col2 and col3.

Using ColSketcher as a Feature Selector in Supervised Learning.

3.3. Visualization

This section presents several multivariate visualizations that are particularly suited to our matrix sketching algorithm on rows and columns of the data matrix.

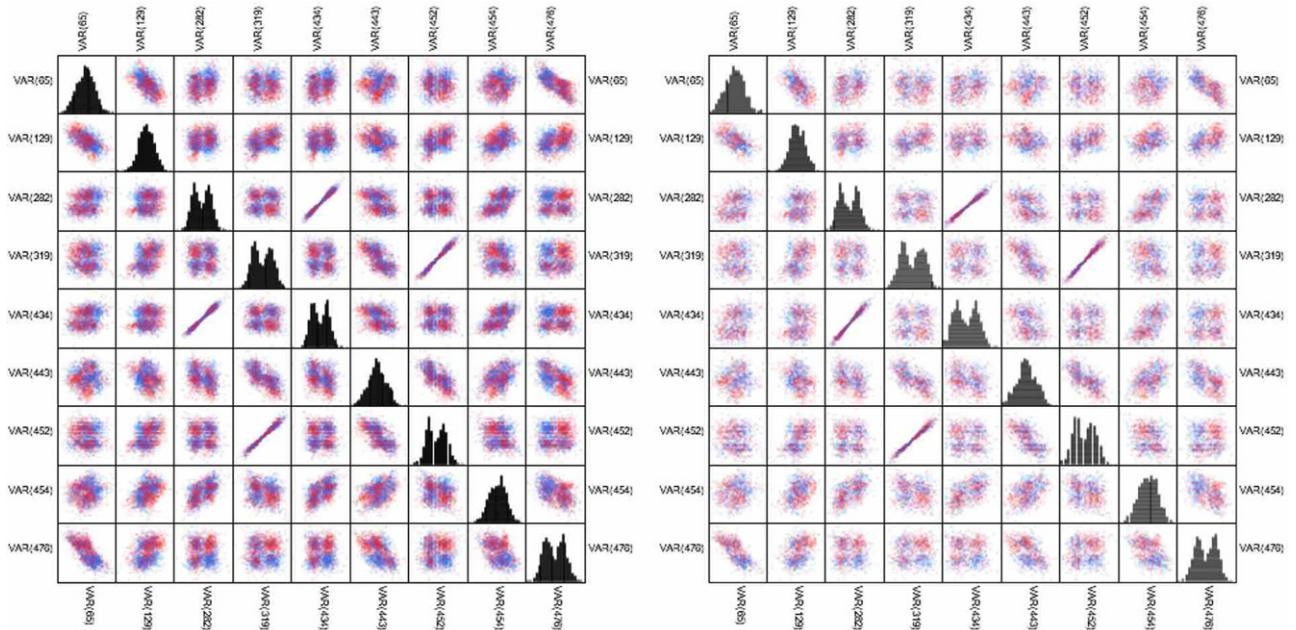


Figure 10. SPLOM on 2000 Madelon rows (left) and 1000 (right), 500 columns reduced to 10. The tenth variable (CLASS) is used to color the scatterplots.

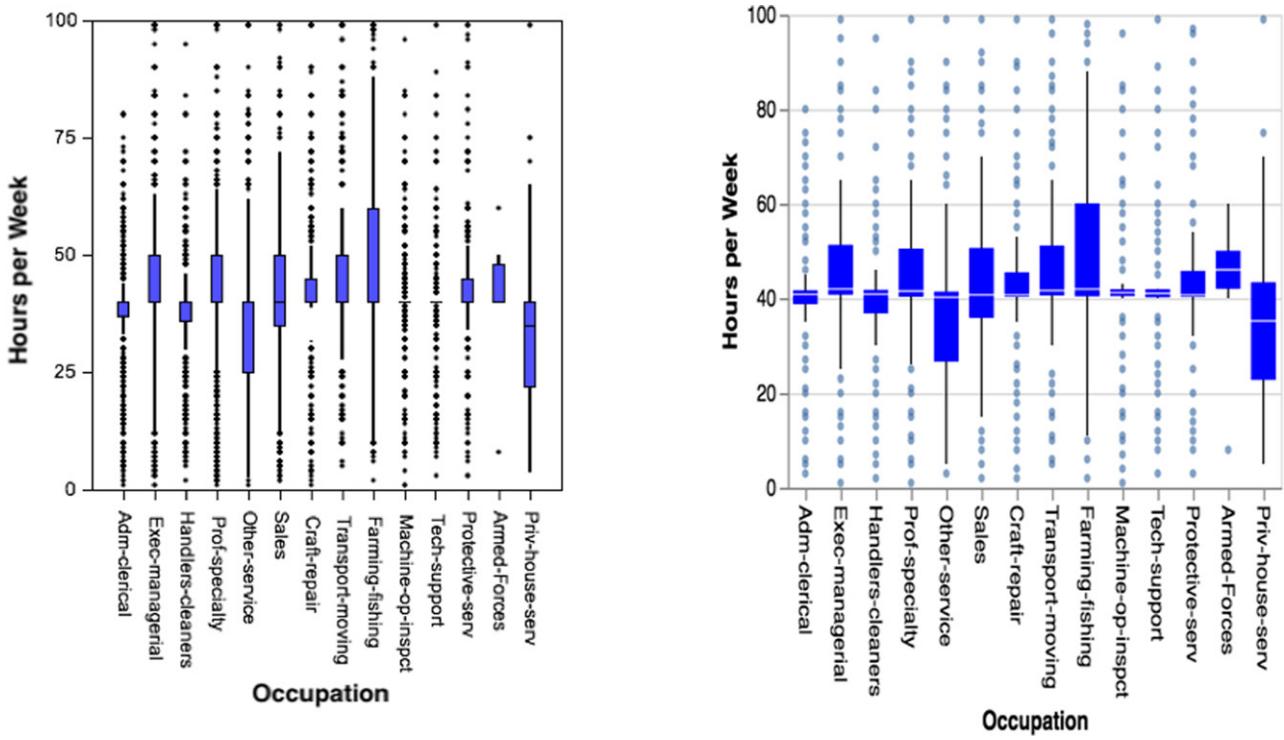


Figure 11. Full adult dataset boxplot (left, $N = 32,000$) and row sketched adult dataset boxplot (right, $n = 430$).

3.3.1. Biplots

Figure 7 shows a biplot (Gabriel 1971) of the Madelon training dataset (Guyon et al. 2007). We reduced 2000 rows to 1000 and 500 columns to 20. This biplot represents principal component loadings with vectors (red) and scores with points (blue)—all in the same frame. The biplot in the left panel obscures most of the variation in cases and variables. The biplot in the right panel shows the 20 vectors representing

the column variables. The canonical correlation between the coordinates of the vectors in the right plot with the coordinates of the corresponding vectors in the left plot is 0.89. This indicates that the right plot is accurately representing the relevant loadings in the principal components of the full dataset. In addition, the sketch plot spans the full 2D space the way the full-data plot does. It is not a seriously biased representation.

3.3.2. Parallel Coordinates

Parallel Coordinates, in various forms, are one of the most popular multidimensional visual analytic methods for big data (Johansson et al. 2005; Inselberg 2009; Zhang and Huang 2016). Their well-known weakness is visual clutter, caused both by many cases and many variables. Obvious remedies for this problem include the use of kernels, profile aggregation, and sorting of variables to reduce crossings. Our sketching algorithm on rows and columns makes all these remedies easier to realize, especially with limited computational resources.

Figure 8 shows parallel coordinates using our sketching algorithm on rows and columns on a popular dataset comprising delays in air traffic performance (https://www.transtats.bts.gov/OT_Delay/OT_DelayCause1.asp). A k -means cluster analysis is used to color the display, which clearly reveals two different clusters (Caliński and Harabasz 1974) on the performance variables. The panel on the left is the plot before sketching. The clusters are not salient because of the overall scale and there is considerably more clutter.

3.3.3. Heatmaps

Cluster heatmaps involve joint reorderings of the rows and columns of a data matrix using hierarchical clustering (Wilkinson and Friendly 2009). They are impractical for big data for two reasons. First, display resolution prevents the rendering of cells in large heatmaps, even when cells are depicted in single pixels. Second, the number of rows and/or columns in big data matrices exceeds the computational efficiency of hierarchical clustering. Matrix sketching is suited as a remedy for these problems.

Figure 9 shows a cluster heatmap of gene expression data using matrix sketching. The data are from Weinstein et al. (2013), see also Khomtchouk et al. (2017). We reduced 801 rows and 20,531 columns to 47 rows and 40 columns. The display indicates joint clusters (particularly in the lower left) that might be fruitful for further analysis.

3.3.4. Scatterplot Matrices

Figure 10 shows a scatterplot matrix on sketched columns of the Madelon dataset (Guyon et al. 2007). There are two interesting aspects of these plots. First, the sketched columns reveal anomalous artificial structures embedded in this dataset. In particular, the two straight-line relationships between columns clearly stand out against the other patterns. These are the only anomalous ones of this kind in the whole dataset. Sketching is not an anomaly detector, but when embedded among relatively homogeneous distributions, anomalous relations are likely to be exposed. Columns on which there are outliers, for example, will have more leverage in the distance correlation calculations. Second, the two SPLOMs are remarkably similar.

3.3.5. Boxplots

Figure 11 shows a Tukey schematic (boxplot) for the U.S. Census Adult dataset (<https://archive.ics.uci.edu/ml/datasets/adult>). The plot on the left is for the complete dataset and the one on the right is derived from the row sketch of the same dataset. Despite a nearly 75% reduction in the number of cases, the two plots are visually almost indistinguishable. Furthermore,

the row sketched boxplot outliers are brushable as long as the members indices are retained as pointers.

4. Conclusion

In a landmark paper relatively unknown to many computer scientists and statisticians today, Amos Tversky discussed the use of real vector spaces in data science (Tversky 1977). At the time of the paper, psychologists were enthusiastic about the possibility of using multidimensional scaling (*MDS*) to derive a cognitive map (points in a metric space) from judgments of the similarities between objects. Tversky demonstrated that some types of data are inappropriate for methods that depend on metric axioms. A simple example is the triad of statements most observers would agree with:

- Miami is similar to Havana
- Havana is similar to Moscow
- But Miami is not similar to Moscow

Tversky argued against the indiscriminate use of metric space models in psychology, but there is perhaps a wider range of indiscriminate usage of nonlinear manifold models in machine learning and visualization today. Users of these methods may assume that they are appropriate for any numerical data.

A corollary of Tversky's observation, in the context of today's multidimensional visualization practices, might be our point in the Related Work section that visualizations that violate metric axioms can be harmful, leading viewers to misinterpret similarities between objects. Judging dissimilar points as similar or similar points as dissimilar can lead to false conclusions. Today's popular multidimensional visualization algorithms are not intrinsically flawed; their flaws lie in their indiscriminate uses that do not take into account the assumptions underlying them.

In addition to the primary motivation for this research (distance-preservation under projections), there is a significant concomitant benefit. It involves reification of composites. As Drineas, Mahoney, and Muthukrishnan (2008) point out,

Although the truncated SVD is widely used, the vectors u^i and v^i themselves may lack any meaning in terms of the field from which the data are drawn. For example, the eigenvector

$[(1/2)\text{age} - (1/\sqrt{2})\text{height} + (1/2)\text{income}],$ being one of the significant uncorrelated "factors" or "features" from a dataset of people's features, is not particularly informative or meaningful. This fact should not be surprising. After all, the singular vectors are mathematical abstractions that can be calculated for any data matrix. They are not "things" with a "physical" reality.

Nevertheless, data analysts often fall prey to a temptation for reification, that is, for assigning a physical meaning or interpretation to all large singular components.

Drineas, Mahoney, and Muthukrishnan (2008) explain axis-parallel representation as a strength of the CUR decomposition.

We agree. While our algorithm is fundamentally different from theirs, it shares interpretive advantages with CUR.

We do not propose that our sketching algorithm on rows and columns replace other methods for handling big data problems. Each method has its own advantages. Our algorithm on rows and columns has several, each designed to facilitate visual analysis of large datasets. First, it returns a subset of a given matrix, not a set of additive composites. This facilitates brushing and linking to real data values rather than to composites. Second, our algorithm is more scalable than other projection methods, especially iterative ones like manifold learning or projection pursuit. And, finally, our algorithm is distance-preserving so that the resulting low-dimensional visualizations are less likely to violate the metric axioms when we use sketching inside the visualization flow running from data to perceived structures, patterns, and relationships.

Supplementary Materials

Supporting materials, including source code, are available at <https://github.com/hrluo/DistancePreservingMatrixSketch>. Wilkinson devised the row and column algorithms, wrote the main section of the article, coded the Java applications and the dataset evaluations. Luo devised the proofs, wrote the Appendix, coded the R and Python versions, and edited the article.

Acknowledgments

We are grateful to the editor, the AE, and two anonymous reviewers for constructive comments and suggestions that have significantly improved the article.

References

- Ali, S., Gupta, N., Nayak, G., and Lenka, R. (2016), "Big Data Visualization: Tools and Challenges," in *2016 2nd International Conference on Contemporary Computing and Informatics (IC3I)*. IEEE. [946]
- Asimov, D. (1985), "The Grand Tour: A Tool for Viewing Multidimensional Data," *SIAM Journal on Scientific and Statistical Computing*, 6, 128–143. [948]
- Batch, A., and Elmquist, N. (2017), "The Interactive Visualization Gap in Initial Exploratory Data Analysis," *IEEE Transactions on Visualization and Computer Graphics*, 24, 278–287. [945]
- Belkin, M., and Niyogi, P. (2003), "Laplacian Eigenmaps for Dimensionality Reduction and Data Representation," *Neural Computation*, 15, 1373–1396. [949]
- Calinski, T., and Harabasz, J. (1974), "A Dendrite Method for Cluster Analysis," *Communications in Statistics-Simulation and Computation*, 3, 1–27. [947,957]
- Carr, D., Kahn, R., Sahr, K., and Olsen, A. R. (1997), "ISEA Discrete Global Grids," *Statistical Computing and Graphics Newsletter*, 8, 31–39. [948]
- Carr, D. B., Littlefield, R. J., Nicholson, W. L., and Littlefield, J. S. (1987), "Scatterplot Matrix Techniques for Large n," *Journal of the American Statistical Association*, 82, 424–436. [948]
- Cavallo, M., and Demirpal, C. (2018), "A Visual Interaction Framework for Dimensionality Reduction based Data Exploration," in *Extended Abstracts of the 2018 CHI Conference on Human Factors in Computing Systems*, CHI EA '18, New York, NY, USA. Association for Computing Machinery. [948]
- Cheng, C. H., Fu, A. W., and Zhang, Y. (1999), "Entropy-Based Subspace Clustering for Mining Numerical Data," in *KDD '99*. [948]
- Cormode, G., and McGregor, A. (2008), "Approximation Algorithms for Clustering Uncertain Data," *PODS '08*, 191–200. [949]
- Cutura, R., Aupetit, M., Fekete, J.-D., and Sedlmair, M. (2020), "Comparing and Exploring High-dimensional Data with Dimensionality Reduction Algorithms and Matrix Visualizations," in *Proceedings of the International Conference on Advanced Visual Interfaces*, pp. 1–9. [953]
- Ding, C., and He, X. (2004a), "Cluster Structure of k-means Clustering via Principal Component Analysis," in *PAKDD 2004: Advances in Knowledge Discovery and Data Mining*, pp. 414–418. Springer. [947]
- (2004b), "K-means Clustering via Principal Component Analysis," in *ICML '04: Proceedings of the Twenty-First International Conference on Machine Learning*, pp. 6–15. IEEE. [947]
- Drineas, P., Kannan, R., and Mahoney, M. W. (2006), "Fast Monte Carlo Algorithms for Matrices iii: Computing a Compressed Approximate Matrix Decomposition," *SIAM Journal on Computing*, 36, 184–206. [951]
- Drineas, P., Mahoney, M. W., and Muthukrishnan, S. (2008), "Relative-Error CUR Matrix Decompositions," *SIAM Journal on Matrix Analysis and Applications*, 30, 844–881. [949,957]
- DuMouchel, W. (2002), "Data Squashing: Constructing Summary Data Sets," in *Handbook of Massive Data Sets: Massive Computing*, eds. J. Abello, P. Pardalos, and M. Resende, pp. 579–591, Boston: Springer. [947]
- DuMouchel, W., Volinsky, C., Johnson, T., Cortes, C., and Pregibon, D. (1999), "Combining Automated Analysis and Visualization Techniques for Effective Exploration of High-dimensional Data," in *Proceedings of the Fifth ACM Conference on Knowledge Discovery and Data Mining*, pp. 6–15. IEEE. [947]
- Dy, J., and Brodley, C. (2004), "Feature Selection for Unsupervised Learning," *Journal of Machine Learning Research*, 5, 845–889. [948]
- Fekete, J., and Plaisant, C. (2002), "Interactive Information Visualization of a Million Items," *IEEE Symposium on Information Visualization, 2002. INFOVIS 2002*, pp. 117–124. [946]
- Friedman, J., and Meulman, J. (2004), "Clustering Objects on Subsets of Attributes," *Journal of the Royal Statistical Society*, 66, 815–849. [948]
- Gabriel, K. (1971), "The Biplot Graphical Display of Matrices with Application to Principal Component Analysis," *Biometrika*, 58, 453–467. [956]
- Greenacre, M. (1984), *Theory and Applications of Correspondence Analysis*, London: Academic Press. [950]
- Greenacre, M., and Blasius, J. (2006), *Multiple Correspondence Analysis and Related Methods*, Boca Raton, FL: Chapman & Hall/CRC. [950]
- Guyon, I., Gunn, S., Nikravesh, M., and Zadeh, L. A. (2006), *Feature Extraction: Foundations and Applications (Studies in Fuzziness and Soft Computing)*, Berlin: Springer-Verlag. [946,948]
- Guyon, I., Li, J., Mader, T., Pletscher, P. A., Schneider, G., and Uhr, M. (2007), "Competitive Baseline Methods Set New Standards for the NIPS 2003 Feature Selection Benchmark," *Pattern Recognition Letters*, 28, 1438–1444. [956,957]
- Halko, N., Martinsson, P., and Tropp, J. (2011), "Finding Structure with Randomness: Probabilistic Algorithms for Constructing Approximate Matrix Decompositions," *SIAM Review*, 53, 217–288. [949]
- Hartigan, J. (1975), *Clustering Algorithms*, New York: Wiley. [949,950]
- Hotelling, H. (1933), "Analysis of a Complex of Statistical Variables into Principal Components," *Journal of Educational Psychology*, 24, 417–441. [948]
- Hsieh, W. (2009), "Nonlinear Principal Component Analysis," in *Artificial Intelligence Methods in the Environmental Sciences*, eds. S. E. Haupt, A. Pasini, and C. Marzban, pp. 173–190, Dordrecht: Springer. [948]
- Hurley, C., and Oldford, R. (2011), "Pairwise Display of High-Dimensional Information via Eulerian Tours and Hamiltonian Decompositions," *Journal of Computational and Graphical Statistics*, 19, 861–886. [948]
- Inselberg, A. (2009), *Parallel Coordinates: Visual Multidimensional Geometry and its Applications*, New York: Springer-Verlag. [957]
- Johansson, J., Ljung, P., Jern, M., and Cooper, M. (2005), "Revealing Structure Within Clustered Parallel Coordinates Displays," in *INFOVIS 2005: IEEE Symposium on Information Visualization*, pp. 125–132. IEEE. [957]
- Keim, D. (2000), "Designing Pixel-Oriented Visualization Techniques: Theory and Applications," *IEEE Transactions on Visualization and Computer Graphics*, 6, 59–78. [945]
- Khomtchouk, B. B., Hennessy, J. R., and Wahlestedt, C. (2017), "shiny-heatmap: Ultra Fast Low Memory Heatmap Web Interface for Big Data Genomics," *Plos One*, 12, e0176334. [957]



- Kimerling, J. A., Sahr, K., White, D., and Song, L. (1999), "Comparing Geometrical Properties of Global Grids," *Cartography and Geographic Information Science*, 26, 271–288. [948]
- Kosugi, Y., Ikebe, J., Shitara, N., and Takakura, K. (1986), "Graphical Presentation of Multidimensional Flow Histogram Using Hexagonal Segmentation," *Cytometry*, 7, 291–294. [948]
- Krause, J., Dasgupta, A., Fekete, J.-D., and Bertini, E. (2016), "Seekaview: An Intelligent Dimensionality Reduction Strategy for Navigating High-dimensional Data Spaces," in *2016 IEEE 6th Symposium on Large Data Analysis and Visualization (LDAV)*. IEEE. [946, 948]
- Kruskal, J. (1964), "Multidimensional Scaling by Optimizing Goodness of Fit to a Nonmetric hypo0," *Psychometrika*, 29, 1–27. [948]
- Liberty, E. (2013), "Simple and Deterministic Matrix Sketching," in *Proceedings of the 19th ACM SIGKDD International Conference on Knowledge Discovery and Data Mining*, KDD '13, New York, NY, USA, pp. 581–588. Association for Computing Machinery. [949]
- Luo, H., Patania, A., Kim, J., and Vejdemo-Johansson, M. (2020), "Generalized Penalty for Circular Coordinate Representation." arXiv:2006.02554, 1–39. [945, 948]
- Mahajan, M., Nimborkar, P., and Varadarajan, K. (2009), "The Planar k-means Problem is np-Hard," in *International Workshop on Algorithms and Computation*, pp. 274–285. Springer. [947]
- McInnes, L., Healy, J., and Melville, J. (2018), "UMAP: Uniform Manifold Approximation and Projection for Dimension Reduction." <https://arxiv.org/abs/1802.03426> [949]
- Pahins, C., Stephens, S., Scheidegger, C., and Comba, J. (2016), "Hashed-cubes: Simple, Low Memory, Real-Time Visual Exploration of Big Data," *IEEE Transactions on Visualization and Computer Graphics*, 23, 671–680. [948]
- Paradis, E. (2018), "Multidimensional Scaling with Very Large Datasets," *Journal of Computational and Graphical Statistics*, 27, 935–939. [953]
- Park, H., Jeon, M., and Rosen, J. (2003), "Lower Dimensional Representation of Text Data Based on Centroids and Least Squares," *BIT Numerical Mathematics*, 43, 427–448. [947]
- Pearson, K. (1901), "On Lines and Planes of Closest Fit to Systems of Points in Space," *Philosophical Magazine*, 2, 559–572. [948]
- Peña, L. E. V., Mazahua, L. R., Hernández, G. A., Zepahua, B. A. O., Camarena, S. G. P., and Cano, I. M. (2017), "Big Data Visualization: Review of Techniques and Datasets," in *2017 6th International Conference on Software Process Improvement (CIMPS)*, pp. 1–9. IEEE. [946]
- Rosario, G. E., Rundensteiner, E. A., Brown, D. C., Ward, M. O., and Huang, S. (2004), "Mapping Nominal Values to Numbers for Effective Visualization," *Information Visualization*, 3, 80–95. [950]
- Rousseeuw, P. (1987), "Silhouettes: A Graphical Aid to the Interpretation and Validation of Cluster Analysis," *Journal of Computational and Applied Mathematics*, 20, 53–65. [947]
- Roweis, S. T., and Saul, L. K. (2000), "Nonlinear Dimensionality Reduction by Locally Linear Embedding," *Science*, 290, 2323–2326. [949]
- Sayood, K. (2012), *Introduction to Data Compression* (4th ed.), New York: Morgan-Kaufmann. [948]
- Shepard, R., and Carroll, J. (1966), "Parametric Representation of Nonlinear Data Structures," in *Multivariate Analysis*, ed. P. Krishnaiah, pp. 561–592, New York: Academic Press. [949]
- Shepard, R. N. (1962a), "The Analysis of Proximities: Multidimensional Scaling with an Unknown Distance Function. I," *Psychometrika*, 27, 125–139. [948]
- (1962b), "The Analysis of Proximities: Multidimensional Scaling with an Unknown Distance Function. II," *Psychometrika*, 27, 219–246. [948]
- Stewart, G. W., and Stewart, G. W. (1998), "Four Algorithms for the Efficient Computation of Truncated Pivoted QR Approximations to a Sparse Matrix," *Numerische Mathematik*, 83, 313–323. [949]
- Tatu, A., Albuquerque, G., Eisemann, M., Bak, P., Theisel, H., Magnor, M., and Keim, D. (2011), "Automated Analytical Methods to Support Visual Exploration of High-dimensional Data," *IEEE Transactions on Visualization and Computer Graphics*, 17, 584–597. [948]
- Tenenbaum, J. B., de Silva, V., and Langford, J. C. (2000), "A Global Geometric Framework for Nonlinear Dimensionality Reduction," *Science*, 290, 2319–2323. [949]
- Tversky, A. (1977), "Features of Similarity," *Psychological Review*, 84, 327–352. [957]
- Unwin, A., Theus, M., and Hofmann, H. (2007), *Graphics of Large Datasets: Visualizing a Million*, New York: Springer-Verlag. [946]
- van der Maaten, L., and Hinton, G. (2008), "Visualizing High-dimensional Data Using t-SNE," *Journal of Machine Learning Research*, 9, 2579–2605. [949]
- Wattenberg, M., Viégas, F., and Johnson, I. (2016), "How to Use t-SNE Effectively," *Distill*. <https://distill.pub/2016/misread-tsne/> [949]
- Weinstein, J. N., Collisson, E. A., Mills, G. B., Shaw, K. R. M., Ozenberger, B. A., Ellrott, K., Shmulevich, I., Sander, C., Stuart, J. M., and The Cancer Genome Atlas Research Network. (2013), "The Cancer Genome Atlas Pan-cancer Analysis Project," *Nature genetics*, 45, 1113–1120. [957]
- Wilkinson, L. (1999), "Dot Plots," *The American Statistician*, 53, 276–281. [947]
- Wilkinson, L., and Friendly, M. (2009), "The History of the Cluster Heat Map," *The American Statistician*, 63, 179–184. [957]
- Xie, Y., Chenna, P., He, J., Le, L., and Planteen, J. (2009), "Combining Automated Analysis and Visualization Techniques for Effective Exploration of High-dimensional Data," in *2009 IEEE Symposium on Visual Analytics Science and Technology*. IEEE. [948]
- Xie, Y., Chenna, P., He, J., Le, L., and Planteen, J. (2016), "Visualization of Big High Dimensional Data in a Three Dimensional Space," in *2016 IEEE/ACM 3rd International Conference on Big Data Computing Applications and Technologies (BDCAT)*. IEEE. [947]
- Zhang, J., and Huang, M. (2016), "2D Approach Measuring Multidimensional Data Pattern in Big Data Visualization," *2016 IEEE International Conference on Big Data Analysis (ICBDA)*, 1–6. [957]
- Zou, H., Hastie, T., and Tibshirani, R. (2006), "Sparse Principal Components," *Journal of Computational and Graphical Statistics*, 15, 265–286. [948]