Using Distance Metrics to Examine How Subjects Read Data Plots in a Large Amazon Turk Study

Abstract

Graphics play a crucial role in statistical analysis and data mining. Being able to quantify structure in data that is visible in plots, and how people read the structure from plots is an ongoing challenge. This paper describes metrics developed to assist with this, and utilizes them to evaluate how people select plots from lineups used for visual inference. Lineups embed the plot of the data among a set of null plots, and engage a human observer determine whether the data plot is different from the nulls. The data plot is treated like a test statistic, and protocol acts like a comparison with the sampling distribution of the nulls. Metrics are calculated in association with lineups to help understand what people see in the data plots, and assess the quality of a lineup, because the null plots represent a finite sample from a null distribution, and this finiteness may affect how observers read the lineups. The distance metrics are designed to describe how different the data plot is from the null plots, and the null plots from each other. Analysis of the distance metrics was conducted on data collected through a large number of Amazon Turk studies that have used the lineup protocol for studying an array of data analysis tasks.

Keywords: data visualization, statistical graphics, data mining, data science, information visualization

things to do:

- reduce paper to 30 pages + appendix (from 40 pages + 3 pages of appendix): strategy: explain first example in detail, include only conclusions for the other two examples, put supporting material into the appendix Di suggests the intro could be reduced, remove the Tukey quote, tighten up the distance descriptions but keep the plots, maybe fig 7, fig 14 could be moved to appendix
- restructure introduction: include findings from previous studies, such as permutation-invariance; include description of how data is collected;
- be more precise in lineup description: null hypotheses
- add citations (Marron and Tsybakov, 1995) and (Hannig et al., 2013) in the text
- title change
- conclusions don't match results, the specialist metric does not always ourperform the binned

1 Introduction

Graphics are an important component of big data analysis, providing a mechanism for discovering unexpected patterns in data. Pioneering research by Gelman (2004), Buja et al. (2009) and Majumder et al. (2013) provide methods to quantify the significance of discoveries made from visualizations. Buja et al. (2009) introduced two protocols, the Rorschach and the lineup protocol, which bridge the gulf between traditional statistical inference and exploratory data analysis. The Rorschach protocol consists of a set of m (usually, $m = 20$) plots (called the *null plots*) rendered from data that is consistent with a given null model. That way, the Rorschach protocol helps to understand the extent of randomness in the null model. Under the lineup protocol, a plot of the observed data is placed randomly among a set of $m - 1$ null plots. Human observers are then asked to examine the lineup and to identify the most different plot. If observers identify the data plot, this is quantifiable evidence against the null hypothesis. The lineup protocol places a statistical plot firmly in the framework of hypothesis tests: a plot of the data is considered to be the test statistic, which is compared against the sampling distribution under the null hypothesis represented by the null plots. Obviously, the null generating mechanism, i.e. the method of obtaining the data for null plots, is crucial for both the lineup and the Rorschach protocol. The null hypothesis directly affects the choice of null generating method. Null generating methods are typically based on (a) simulation, if the null hypothesis allows us to directly specify a parametric model, (b) sampling, as for example in the case of large data sets, or (c) permutation of the original data (see e.g. Good, 2005), which allows for non-parametric testing that preserves marginal distributions while ensuring independence in higher dimensions.

The lineup protocol was formally tested in a head-to-head comparison with the equivalent conventional test in Majumder et al. (2013). The experiment utilized human subjects from Amazon's Mechanical Turk (Amazon, 2005-2015) and used simulation to control conditions. The results suggest that visual inference is comparable to conventional tests in a controlled conventional setting. This provides support for its appropriateness for testing in real exploratory situations where no conventional test exists. Interestingly, the power of a visual test increases with the number of observers engaged to evaluate lineups, and

the pattern in results suggests that the power will provide results consistent with practical significance (Kirk, 1996).

Figure 1 gives an example of one of the lineups used in a head-to-head comparison with classical testing (results are discussed in more detail in section 3.2). Suppose we have the

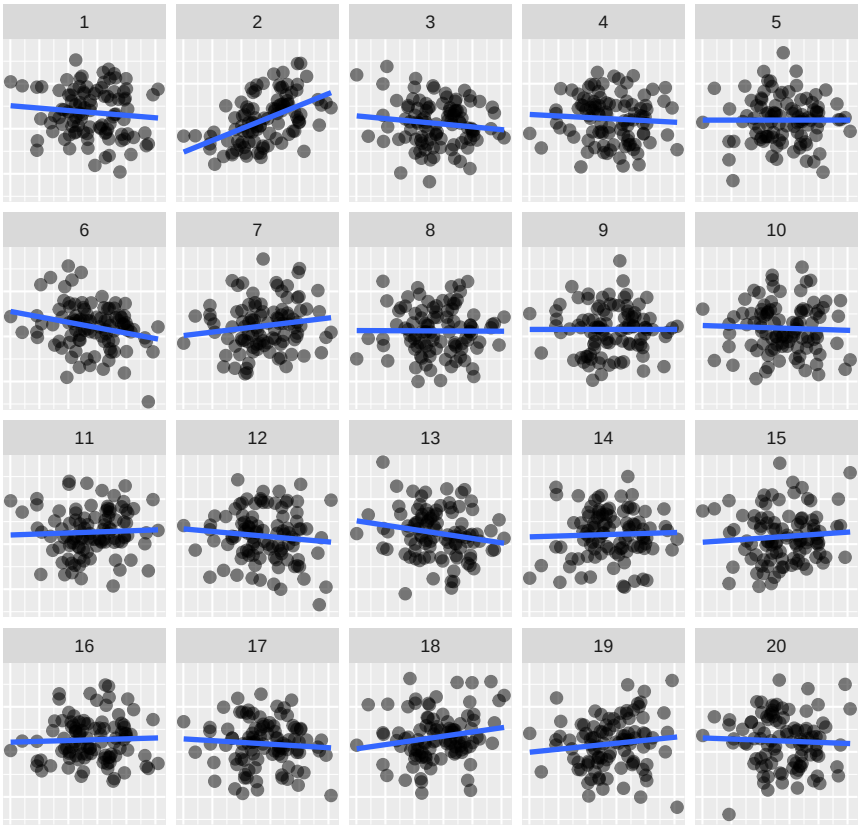


Figure 1: Lineup plot of size $m = 20$ of scatterplots with overlaid regression line. This tests $H_o : \beta_k = 0$, where covariate X_k is continuous. One of the plots in the lineup is the plot of the true data. The other plots are null plots generated by simulating data from a null model that assumes that the null hypothesis is true. Can you identify the plot with the steepest slope?

following statistical model

$$Y_i = \beta_0 + \beta_1 X_{i1} + \beta_2 X_{i2} + \cdots + \epsilon_i$$

and we are interested in testing the following hypothesis:

$$H_o : \beta_k = 0 \qquad \text{vs} \qquad H_A : \beta_k \neq 0$$

where X_k is a continuous covariate. Assume, the data plot is a scatterplot of Y against X_k with a regression line overlaid. We can generate null plots from rendering simulating data from $N(X\hat{\beta}, \hat{\sigma}^2)$ and plotting using the same scatterplot method as the true data, where parameter estimates $(\hat{\beta}, \hat{\sigma}^2)$ are obtained by fitting the null model to the true data.

The plot of the true data is randomly placed among a set of (m - 1) null plots to produce a lineup of size m. Rather than to identify the most different plot, human subjects are asked to identify the plot with the steepest slope from the lineup of Figure 1. If the human subjects can identify the plot of the true data, we reject the null hypothesis and conclude that there is a significant linear relationship between Y and X_k. For the example of this lineup 66 out of 70 observers correctly identify plot #2 as the data plot, providing very strong evidence of a linear relationship.

In traditional hypothesis testing, the sampling distribution of a test statistic is functional and continuous. In the lineup protocol, although conceptually we may have an infinite collection of plots from the null distribution, in practice, we can only evaluate against a finite number of null plots. A human judge has a physical limit on the number of plots they can peruse. This poses one of the issues with using the lineup protocol. Figure 2 illustrates the difference. In traditional inference, the black curve represents the sampling distribution for the t-distribution under the null hypothesis, and the shaded red area shows the rejection region.

Plots are used as test statistics in visual inference, which are, unlike their traditional counterparts, not simple numbers but more complex entities. We can, however, calculate the value of the test statistic based on the data underlying the true plot, as well as the corresponding value for each of the null plots. These values are shown using the red bar (data plot) and the blue bars (null plots) in Figure 2. Effectively, in visual inference the red line is compared to only these finite number of blue lines to make a decision, unlike classical inference where we look at the rejection region (Figure 2) to make decisions. Even though the data plot might be extreme, it is possible by randomly selecting from the null distribution, to obtain a null plot that is more extreme, as Tukey suggested (Fernholz, 2003):

> "There [in Tukey's Data Analysis class] I discovered that [...] a random

(a) Classical Inference (b) Visual Inference

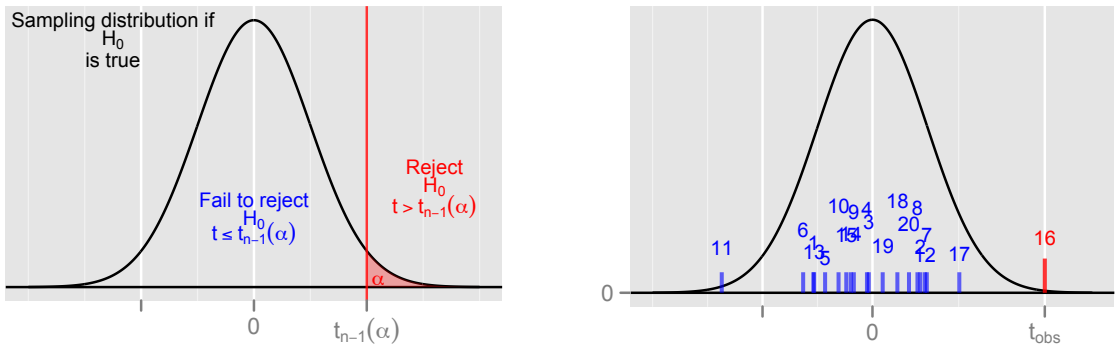


Figure 2: If the lineup protocol was to be used instead of classical inference this is what it would look like. (a) Rejection region (shaded in red) for classical inference for $H_0 : \mu = \mu_0$ vs $H_a : \mu > \mu_0$ and (b) values corresponding to the true value (red) and the null plots (blue) in a single lineup of size $m = 20$ that would be used to test the same null hypothesis. The actual data plot is extreme relative to the null plots, and observers would likely be able to pick it out, resulting in a decision to reject the null hypothesis. In practice, the lineup protocol would not be used if a classical test can be used.

> sample is indeed a "batch of values" which "fail to be utopian" most of the time."

This can be partially solved by having a large number of observers, who each evaluate lineups constructed using different null plots. Having some idea of the type of coverage of the sampling distribution that is provided by the lineups would be useful ahead of engaging observers and evaluating the lineups. Could we say that lineup X is expected to be "difficult" but lineup Y is expected to be "easy"? This information might then help in planning other aspects of the experiment such as e.g. determining an appropriate number of observers. Intuitively, a difficult lineup is one where the data plot is similar to the null plots, while the data plot in an easy lineup has some feature that makes it stand out from the null plots. Being able to compute a distance metric based on features of the plot would be very helpful ahead of running a lineup protocol.

This is a two way process: As metrics are devised to measure the quality of a lineup, the lineup protocol also provides an opportunity to measure the performance of a metric. The human eye can detect patterns in a plot that cannot be easily quantified numerically, which

is why graphics provide an important tool for exploring data and finding the unexpected. Describing plots numerically, is something of an oxymoron, it cannot be universally done. An example of past work are *scagnostics*, short for scatterplot cognostics (Tukey, 1977), which were further investigated in form of graph-based scagnostics (Wilkinson et al., 2005). Both attempt to assess various aspects of scattered points like outliers, shape, trend, density and coherence. If a scatterplot has just one of these structures the scagnostics are descriptive, however, they fail terribly if a plot contains more than one or an unforeseen feature instead. The goal here is to find distance measures that can provide an indication of the quality of a lineup, and then to use the results of observer evaluation to determine which metrics best reflect what features of a plot people see and assess for their choice.

Following up on choices, observers are asked to describe their reasoning. These reasons are used to obtain more information about the rejection: was it some nonlinear dependency, an outlier, clustering or something else that triggered the detection of the data plot? Good distance metrics may also help to relate the descriptive words used to mathematically defined features.

The article is organized as follows. Section 2 starts by defining distance measures and discussing different choices of measures (see Section 2.1). The distribution of the distance measures are studied in Section 2.2. Section 2.3 describes the effect of the plot type and the question of interest on the distance measure while Section 2.4 talks about the distance evaluations. Section 3 presents a comparison of the distance measures to the performance of human subjects in several experiments conducted by Amazon's Mechanical Turk.

2 Measuring Lineups

2.1 Distance Measures

By calculating the "distance" between plots we may be able to determine if a lineup should be easy – if the actual data plot is detectably different from the null plots – and also to better understand what aspect of the plot people use to make their choice. It is not an easy task to measure the difference between plots. Here we examine several possibilities.

The problem could be tackled by considering the data as a reference distribution, and

compare all of the null sets with this reference. Comparing data with a reference probability distribution or comparing two datasets are common statistical tasks. For example, the Kolmogorov-Smirnov test (Stephens, 1974) sorts values in two samples, computes the empirical distribution function of each and compares these two, to determine if the two samples are likely to have come from the same distribution. The Anderson-Darling (Stephens, 1974) and Shapiro-Wilk (Shapiro and Wilk, 1965) tests compare datasets with normal probability distributions. These measure differences between univariate distributions which limits their applicability to distances between plots, generally.

Hausdorff distance (Huttenlocher et al., 1993) has been successfully used for comparing images. It effectively matches points between sets and computes the distances between the matched points. However, for anything but very small number of points the computational cost of the Hausdorff distance prohibits its use. When permutation is the null generating mechanism, Hamming distance (Hamming, 1950) can be used to calculate how different the permutations are, by measuring the minimum number of substitutions it takes to get from one permutation to another.

Alternatively, interpoint distance metrics might be adapted to measure distances between plots. For example, when the purpose is to show differences between groups in a single plot, like side-by-side boxplots, a distance metric that focuses on group separation calculated on each data set might be useful. Bhattacharyya distance (Bhattacharyya, 1946) is widely used in image processing, for feature extraction. This distance, together with various other measures to calculate distances between groups is implemented in the R package `fpc` (Hennig, 2015).

In the analyses of the experimental data of this paper, we used a dual approach: one distance that we employed for all examples is a relatively simple distance based on binned frequencies, which works fairly well in most circumstances. However, it was clear immediately that plot design, and the question asked, has a large impact on how a plot is read, and specific distance metrics designed for specific plot types and tasks are needed. In order to more closely reflect observers' choices in each experiment, we used at least one more distance tailored to each of these special situations. Below is a summary of distance metrics used. For all of these distance measures, let X denote the true dataset with one or two

variables. Let Y denote the null dataset obtained by using an appropriate null generating mechanism.

1. **Binned Distance (BN):** Let X_1 and X_2 be two continuous variables. Let X_1 be divided into p bins and X_2 divided into q bins. We define the cell count matrix $C(X_1, X_2)$ as a $p \times q$ matrix consisting of the binned frequency of the joint distribution of X_1 and X_2, i.e. let the (i, j)-th element of the matrix be the cell count of the number of points in interval i of X_1 and interval j of X_2. The BN distance is defined as

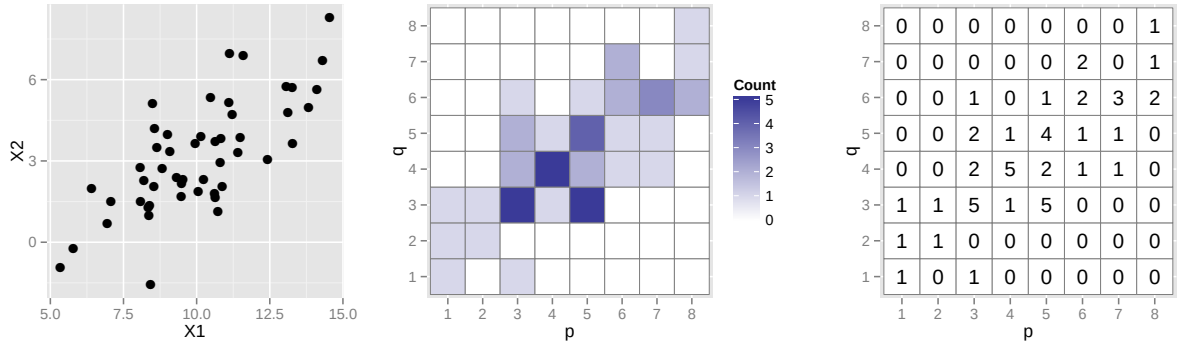
$$\begin{aligned} d^2_{BN}(X, Y) &:= ||C_X(X_1, X_2) - C_Y(X_1, X_2)||^2 \\ &= \sum_{i=1}^{p} \sum_{j=1}^{q} (C_X(X_{1i}, X_{2j}) - C_Y(X_{1i}, X_{2j}))^2. \end{aligned} \tag{1}$$

   This distance can be calculated for univariate continuous data, bivariate data with two categorical variables, or data with one continuous and one categorical variable. For a categorical variable, we choose the number of bins to be equal to the number of categories.

   Binned distance is highly susceptible to small differences in values and depends on the number of bins as well as the anchor point (bottom left corner of cell C_{11}). It is necessary to find the optimal number of bins in each direction. For our purposes 'optimal' was defined as the number of bins that produced the largest detectable difference between observed data plot and null plots, compared to the biggest difference between any pair of null plots. Details of these choices on various different data sets can be found in the Appendix.

   Several variations to this distance are possible, such as a change to using kernel density estimates, a change from L_2 to L_p based distance, or using transformations on the counts. All of these changes will affect distances, and might lead to qualitatively different conclusions. We investigated another generic distance, the Hausdorff distance (Huttenlocher et al., 1993), but the binned distance is computationally much faster to calculate and performed as well as the Hausdorff as a rough, generic measure of similarity of plots.

(a) Dataset X with two variables X_1 and X_2



(b) Dataset Y with permuted X_1 and original X_2

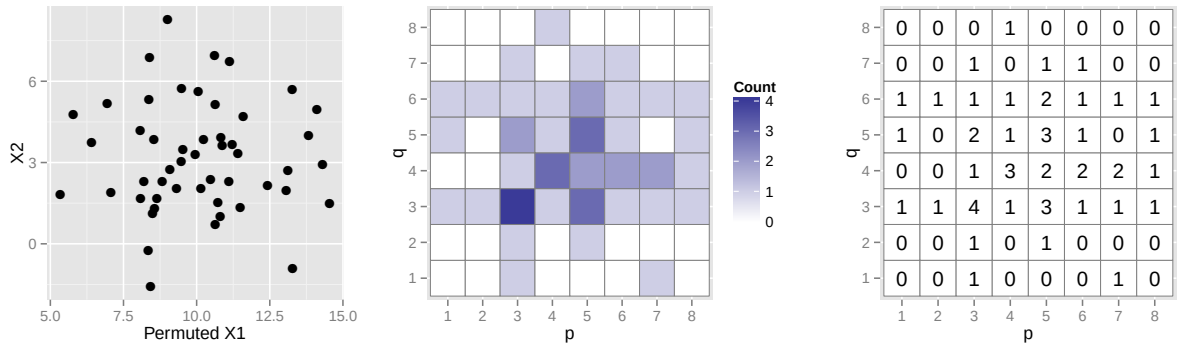


Figure 3: Illustration of binned distance for data with a strong positive association (a), and the same data where variable X_1 has been permuted (b). The scatterplot of the data is shown (left) along with a binned view of the data (center) and the cell count matrix C (right). Binned distance is the Euclidean distance of these counts. The binned distance between these plots is 6.4807.

2. **Distance based on boxplots (BX):** Let X_1 be a categorical variable with J groups and X_2 be a continuous variable. For each of the levels in X_1 find the corresponding X_2 values, and calculate first quartile, median and the third quartile. Identify the minimum and maximum value of each of these statistics across all J groups. Define $d_q(.)$ as a three dimensional vector giving the absolute maximal difference of the first quartile, median and the third quartile of X_2 between the groups in X_1.

   Then the distance metric is given by

$$d^2_{BX}(X,Y) := ||d_q(X) - d_q(Y)||^2 = \sum_{i=1}^{3} \left(d_q(X)_i - d_q(Y)_i\right)^2 .$$

   This distance measure works specifically for boxplots and is based on only their graphical elements. It is based on the assumption that subjects only consider the difference in the boxes to make the distinction. Variations on this might include adding whiskers' values, the number or values of outliers, or including higher-order letter values (Tukey, 1977; Hofmann et al., 2015) for more exact tail specifications.

3. **Distance based on the regression line (RG):** Many times, to examine association between two variables a regression line is overplotted on the points of a scatterplot. This distance was developed to help assess if the observer is paying attention to the line or the spread of points. Let X_1 and X_2 be two continuous variables plotted in a scatterplot. We assume that the scatterplot is binned horizontally into b bins to allow for a description of a piece-wise linear relationship between the variables. In each vertical slice, a linear regression model is fitted and the regression coefficients. i.e. intercept and slope are estimated. The distance metric based on the regression coefficients is given as

$$\begin{aligned} d^2_{RG}(X,Y) &:= \text{tr}(B(X) - B(Y))'(B(X) - B(Y)) \\ &= \sum_{i=1}^{b}((b_0(X))_i - (b_0(Y))_i)^2 + \sum_{i=1}^{b}((b_1(X))_i - (b_1(Y))_i)^2 \end{aligned} \tag{2}$$

   where b_0 and b_1 denote the vector of the intercept and slope respectively while b is the number of bins. $B(.)$ is a $b \times 2$ matrix of the regression coefficients where each row represent the intercept and the slope obtained from each bin. The number of bins

have a significant effect on the distance measure. It can be seen that it works best for smaller number of bins like 1 or 2. With larger number of bins (i.e. smaller bin sizes), the regression coefficients are affected by the variability in the data and the signal to noise ratio in the data becomes too low for a reliable detection. Variations might include using slope alone, or absolute value of slope. Note that we assume that X_1 and X_2 are on the same scale. This does not change the regression or the significance of its parameters, but it does matter for the distance measure. By assuming variables on the same scale, we implicitly expect that the scatterplot has an aspect ratio of 1, which is typically the case in a lineup. This way, a deviation along the x axis is perceived to be about the same as a deviation along the y axis.

4. **Distance based on separation between multiple groups (MS, AS, DS, CM):** Let X_1 and X_2 be two continuous variable. Let X_3 be a categorical variable providing the groups associated with each variable. X_1 and X_2 are plotted in a scatterplot colored by the group variable X_3. The separation can be described in a number of different ways:

   (i) **Minimum separation:** let $s_m(.)$ be a vector of the minimum distance of a point in the cluster to a point in any of the other $g-1$ clusters. The distance metric based on minimal separation is an average of these intercluster minima, defined as

   $$d^2_{MS}(X,Y) := ||s_m(X) - s_m(Y)||^2 = \sum_{i=1}^{g-1}((s_m(X))_i - (s_m(Y))_i)^2.$$

   (ii) **Average point separation:** let $s_a(.)$ be a vector of cluster wise average distances of all the points in a cluster to all points in any of the other $g-1$ clusters. The distance metric based on average separation is defined as

   $$d^2_{AS}(X,Y) := ||s_a(X) - s_a(Y)||^2 = \sum_{i=1}^{g}((s_a(X))_i - (s_a(Y))_i)^2.$$

   (iii) **Dunn separation:** the Dunn index (Dunn, 1973; Halkidi et al., 2001) $s_d(.)$ is defined as the ratio of the minimal separation between clusters and maximal diameter of any of the clusters. The distance metric based on the Dunn index

is defined as

$$d_{DS}^2(X, Y) := (s_d(X) - s_d(Y))^2 .$$

The Dunn index is a member of the Dunn index family, defined as ratios of measures of cluster separation and cluster extent. This makes an analysis of variance approach to clustering, such as Ward's method part of this family as well. Minimal separation between clusters and maximal diameter of a cluster are two very concrete measures. This way, the Dunn index stays close to a visual assessment of the clustering from a cognitive perspective. However, because it is based on two extreme statistics, the Dunn index is highly susceptible to outliers.

We also examined the distance between the means for each cluster (CM) as another alternative, which would more closely match Fisher's linear discriminant. As we might expect, this did not match how observers read the separation. In practice, many possible metrics could be used to measure the separation, such as those readily available in the `fpc` package (Hennig, 2015). Figure 4 illustrates the different distance metrics for cluster separation.

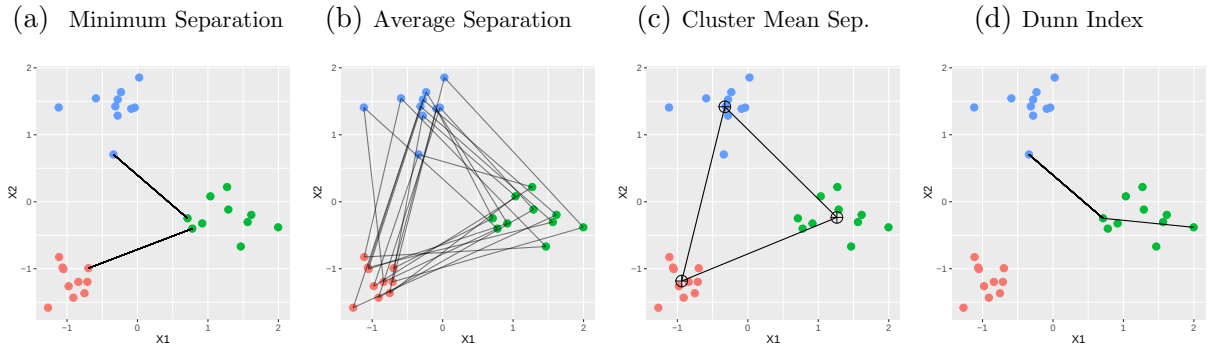


Figure 4: Illustration of four different distance metrics for cluster separation. Minimum Separation (a) calculates the minimum distance between points of each cluster from the other clusters. Average separation (b) calculates the average distance of each point in a cluster to the other clusters. Cluster mean distance (c) sums the distances between the means of each cluster. The Dunn index (d) is based on a comparison of minimal separation between clusters (as shown in (a)) and maximal cluster diameter.

Generally we would expect that different distance measures are not directly comparable

to each other – in order to get an idea of their relative size, we need to find their empirical distribution. This is discussed next.

2.2 Distance Metric Distribution

For a given lineup of size m, the empirical distribution of distance metrics is obtained by calculating the distances between the null plots among themselves. One null data is generated using the null generating mechanism, and labelled to be the "true" data set, then a number of null data sets are generated and the distances between these datasets are calculated. Averaging all these distances yields one single distance value. This process is repeated a large number of times, say, N between 1,000 to 10,000. Finally N mean or average distances are obtained which gives the empirical distribution of the distance. For comparing data plot with nulls using the empirical distribution of the distance metric, we use the following algorithm:

1. Calculate the distance between the true data and all the null datasets and take the average of these distances.
2. For each of the (m - 1) null datasets, calculate the distance between the null data and all the other (m - 2) null datasets and obtain the average distance. Hence, we obtain (m - 1) distances, one corresponding to each null plot.
3. Generate a lineup of size m using the null generating mechanism. Single out one of these nulls as the 'data' plot, and calculate the distances as described in steps (1) and (2). Repeat this procedure N times.
4. The N distance values then represent the empirical distribution of the distance metric and are used for making comparisons

The observed test statistic is compared to the empirical distribution, as shown in Figure 2. The distance measures for the true dataset and the null datasets are plotted on the empirical distribution. If the distance measure of the true plot is larger than any of the null plots, the lineup might be regarded as "easy". Otherwise, we consider it to be a "difficult" lineup. For easy lineups, we would expect that most observers could detect the true data plot amongst the decoys, but that far fewer observers to be able to do so with a difficult

lineup. This gives us a way to compare the actual results from the Turk human subject studies with what we might expect given the distance metric assessment.

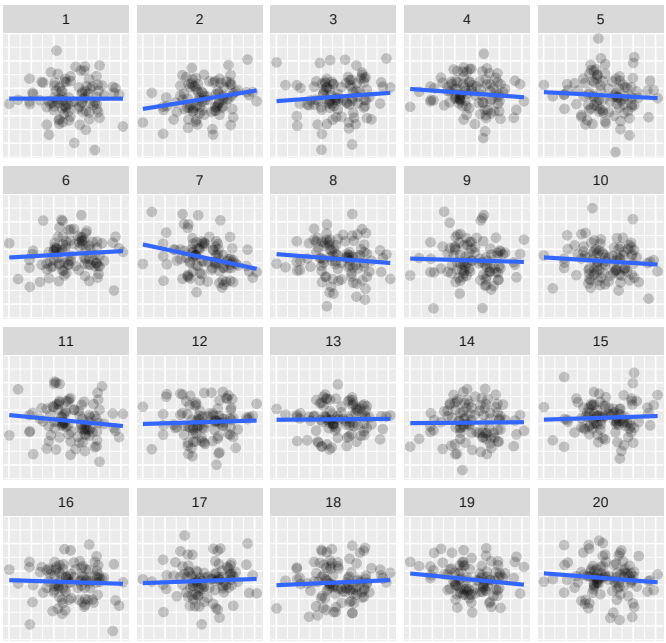
The empirical distribution of the distance based on regression is shown in Figure 5 using $N = 1000$ simulation runs. Figure 5a shows the lineup plot for $m = 20$ for testing whether there exists a significant linear relationship between X_1 and X_2. The 19 null plots are generated by fitting the null model and generating from the null model. Figure 5b shows the general empirical distribution of distance measures based on the null model. For the particular lineup on the left, mean distances are shown by overlaid line segments for the true plot (in orange) and the null plots (in black). The true plot is easily identifiable from the lineup (Figure 5a, in the experiment 40 out of 45 observers identified the data). This is backed by the regression based distance measure seen in Figure 5b, as the orange line is on the extreme right tail compared to the black lines.

Figure 6a shows a lineup of size $m = 20$ for testing whether there exists a significant difference in the group medians between A and B. The 19 null plots are generated from a null model, consisting of draws from a normal distribution. Figure 6b shows the empirical distribution of the distance based on the boxplots with the mean distance for the true plot (in orange) and the null plots (in black). It is hard to identify the true plot from the lineup. During the study, only 2 out of 26 observers picked the data plot, indicating little to no evidence of a deviation from the null hypothesis. This is also evident from the boxplot based distance measure: the orange line corresponding to the true data is mixed in with the mass of the black lines, with one null plot (16) exhibiting a lot more signal than the true plot.

2.3 Effect of Plot Type and Question of Interest

Previous studies have suggested that the type of plot used in the lineup affects the response of the subjects (Hofmann et al., 2012; Zhao et al., 2013). For example, subjects more often identify the true plot for large data with side-by-side box plots than dot plots. Similarly, the use of aesthetics, such as colors or shapes, and graphical elements, such as a trend line, also influence an observer's decision (Vander Plas and Hofmann, 2015). In order to account for this, the distance metric has to be adjusted for the plot type and graphical elements.

(a) Lineup: which slope is the steepest?



(b) Regression based distance metrics.

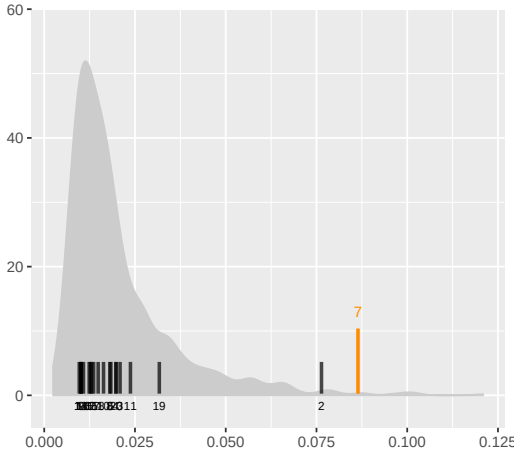
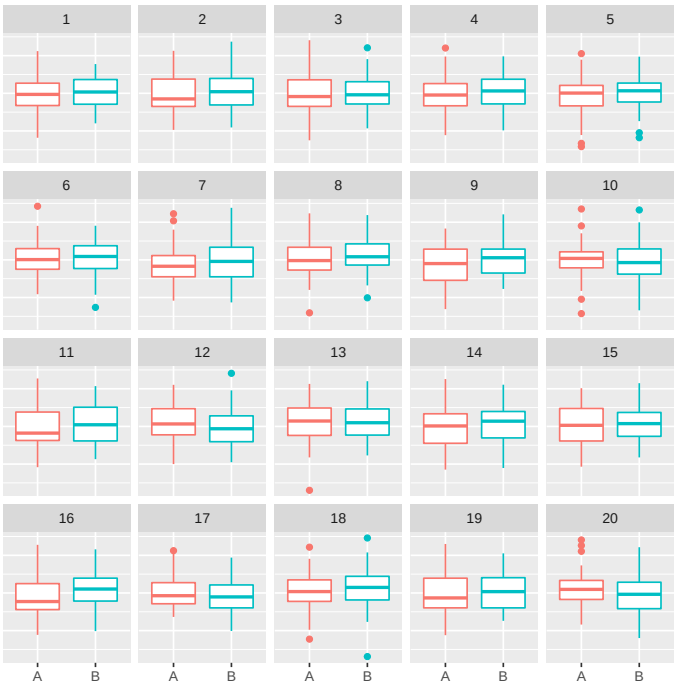


Figure 5: Illustration of the behavior of a distance metric with a lineup plot in (a) and the distribution of regression based distance metric in (b). A lineup of size $m = 20$ is shown (left) for testing whether there exists a significant linear relationship between X_1 and X_2. The 19 null plots are obtained by simulating from the null model. The empirical distribution of the distance metric is shown on the right and overlaid by vertical line segments for the true plot and the null plots (in orange and black, respectively).

(a) Lineup: which of these pairs of boxplots shows the biggest vertical difference?



(b) Boxplot based distance

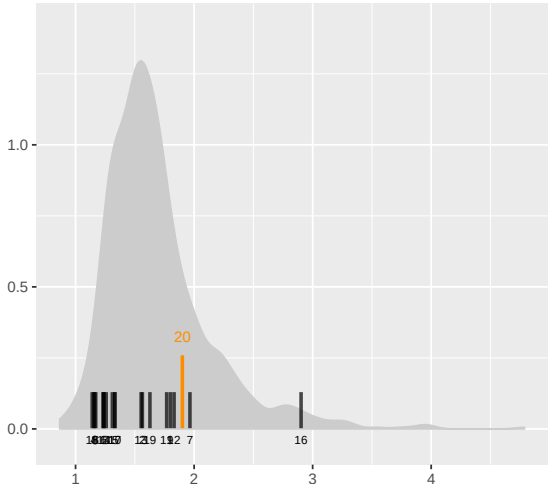


Figure 6: Illustration of the behavior of a distance metric for a more 'difficult' lineup. The lineup is shown in (a), the density plot on the right shows the boxplot based distance metric. Of interest is whether there exists a significant shift between the two groups. The orange line (boxplot distance of the true plot) is among the black lines of the nulls, indicating that the boxes in the true plot show no more difference than a null plot from other null plots.

Figure 7 illustrates this idea.

(a) Lineup of scatterplots

(b) Lineup of scatterplots with trend lines

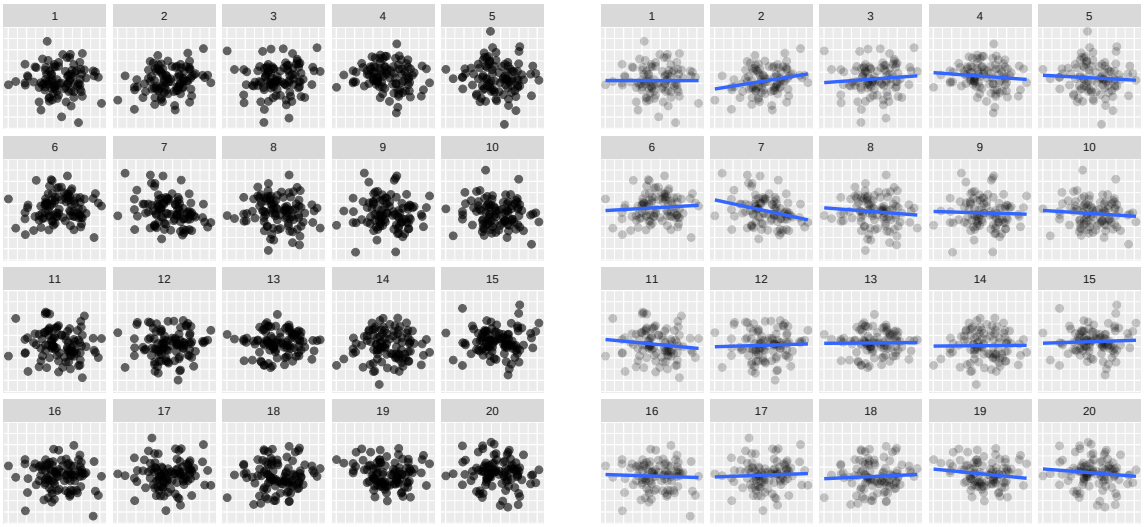


Figure 7: Comparison of two lineups: scatterplots in (a) and scatterplots with a regression line overlaid in (b). The raw data is same for the lineups. The human subjects are shown the lineups and asked to identify the plot with the steepest slope. The presence of the regression line directs the decision of observers.

Figure 7a shows a lineup of scatterplots with 100 points between two variables X_1 and X_2. Figure 7b, on the other hand, gives a lineup of the same scatterplots with the regression line overlaid. The overlaid regression lines are likely to help observers in identifying the panel with the steepest slope. The choice of distance metric depends on what kind of comparisons those distance measures are supposed to allow. Internally, when the same design is used, all measures are consistent – and allow for a relative comparison: an easier lineup will show a bigger positive distance between the true plot and the nulls than a more difficult one. The distance measure does not necessarily allow for an absolute assessment of difficulty. If a distance metric is additionally supposed to assist in planning an experiment where different types of plots are considered or different graphical elements on the same type of plot, the distance metric has to be able to take these differences into account.

The question posed to observers plays an important role in the decision they make. A minor change in the question can change the response of the subject. For example, if subjects are asked to identify a plot from one in the lineups in Figure 7, in which there is the

strongest positive relationship between the variables, plot 2 exhibits the strongest signal. If the question asks, instead, for the plot with the largest slope, plot 7 would be the obvious pick. A distance metric should also take into account the question of interest, and the metrics that we have described in the previous section do this for the MTurk studies done to date where quite specific questions were used. In practice, the question of interest very broad to enable detection of any type of significant structure in a plot, and is generically, "which plot in the lineup is the most different from the others", in which case the binned distance should be optimal.

2.4 Metric Evaluation

For a lineup of size $m = 20$, the average distance of the true plot from all null plots is compared to 18 average distances between the null plots. This high dimensionality of the comparison can sometimes complicate things. A logical solution is to derive a single statistic for each lineup. Such a statistic should take both the mean distance of the true plot into account as well as the maximum of the mean distances for the null plots. Hence we define,

1. **δ-Difference:** let $\bar{d}_{\cdot}$ be the average difference of plot . to all of the (other) null plots. We define the difference between the mean distance for the true plot and the maximum of the mean distances for the null plots as a measure of lineup difficulty, more specifically,

$$\delta(\ell) = \bar{d}_{\text{true}} - \max_{j} \left(\bar{d}_{\text{null}_j}\right) \tag{3}$$

for $j = 1, \ldots, (m-1)$ defines the lineup difference for lineup ℓ. A positive difference indicates that the mean distance of the true plot is larger than the maximum of the mean distances of the null plots. Hence the true plot is more extreme compared to the set of null plots in the lineup. A larger difference should make data plot identification easier. Similarly, a negative difference indicates that there is at least one null plot which is more extreme compared to the true plot based on the distance metric.

However, this statistic does not imply how many null plots are more extreme than the true plot. So we define,

2. **γ-Number of Extreme Nulls:** the number of null plots which have larger mean distances than the mean distance of the true plot is noted. Mathematically, for lineup ℓ, we define the γ-number as

$$\gamma(\ell) = \sum_{j=1}^{m-1} \mathbb{1}\left(\bar{d}_{\text{null}_j} > \bar{d}_{\text{true}}\right), \tag{4}$$

where $\mathbb{1}(.)$ is a zero/one indicator function.

$\gamma(.)$ takes integer values between 0 and $(m-1)$. Higher values indicate more null plots being more extreme than the true plot, making it harder to identify it from the lineup.

Another choice for comparing lineups would be to use empirical p-values from the empirical distribution of the distance metric. While this would enable a comparison of all the metrics for any lineups, this approach is computationally extremely expensive, in particular, because we are generally interested in the extreme values of the empirical distribution, which needs a very large number of simulation runs N for a reliable estimation.

In order to assess how well a distance metric reflects observers' choices, we relate distance metric to the rate at which the data plot in each lineup is being identified. In an ideal scenario, a detection rate of 0.05 corresponds to a δ-difference of zero. With an increase in δ-difference we would expect a simultaneous increase in detection rate. For the evaluation of metrics in the next section, we will fit a logistic regression of detection rate in δ-difference.

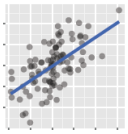
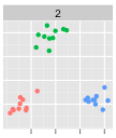
3 Experimental Results and Analysis of Metrics

A number of experiments employing the lineup protocol were run using the MTurk service (Amazon, 2005-2015). A complete list and access to each experiment can be found in Hofmann et al. (2013).

Some experiments are used for evaluating the power of visual inference against that of classical tests (Majumder et al., 2013), some for comparison of different designs (Hofmann et al., 2012; Loy et al., 2015), or for targeted conclusions based on visual inference in situations where traditional tests do not perform well (Yin et al., 2013). In each study, subjects were recruited through the MTurk service and were shown a set of lineups. For

evaluating the distance metrics we used the data collected on three experiments described in Table 1.

Table 1: Overview of the three Turk experiments, from which data was included to investigate distance metrics and how subjects read the plots.

ID	Experiment	Test Statistic	Lineup question
I	Box plot		Which set of box plots shows biggest vertical difference between group A and B? (Majumder et al., 2013)
II	Scatter plot		Of the scatter plots below which one shows data that has steepest slope? (Majumder et al., 2013)
III	Group separation		Which of these plots has the most separation between the coloured groups? (Roy Chowdhury et al., 2015)

We evaluated the performance of the distance metrics in each of the experiments by comparing the distances to the responses from observers.

3.1 Experiment I – Side by Side Boxplots

This study was designed to investigate the power of visual inference in the classical situation of assessing the significance of a co-variate X in a linear model. For the first study, the assumption is that the covariate is discrete (with two levels), while in Experiment II (see section 3.2) we assume the covariate to be continuous. The visual test statistic consists of side-by-side boxplots of the dependent variable against the two levels of covariate X. The data for the lineups comes from a model of the form $y_i + \mu + \beta_{x_i} + \varepsilon_i$ where μ is an overall average, $x_i \in 1, 2$ with $\beta_1 = -\beta_2$ is the effect for each of the two levels of X, and $\varepsilon_i \sim N(0, \sigma^2)$, independent for $i = 1, ..., n$. The null generating mechanism is then a simplified model without the covariate, i.e. $\beta_1 = \beta_2 = 0$. Each of the subjects, recruited through the MTurk service, was asked to evaluate ten lineups, and to identify, in each one,

the plot that exhibits the largest vertical difference between groups A and B. The type of lineup used in this experiment is shown in Figure 6a.

For each lineup, the detection rate is calculated based on the number of evaluations and data identifications by subjects and related to its δ-difference and γ-number of extreme null plots using both the distance based on boxplots (d_{BX}) and the binned distance (d_{BN}, using 8 bins in y direction and 2 in x).

These values are plotted in Figure 8. We see that as δ-difference increases, detection rate generally increases. The solid lines in Figure 8a are fits from logistic regression models using a quadratic effect for distance. The fitted lines come very close to the non-parametric smooth shown by the dashed line. Qualitatively, both boxplot based distance and binned distance show very similar fits for detection rate. Based on the logistic regressions, boxplot distance is fitting detection rate a bit better (AIC: 798.7) than binned distance (AIC: 826).

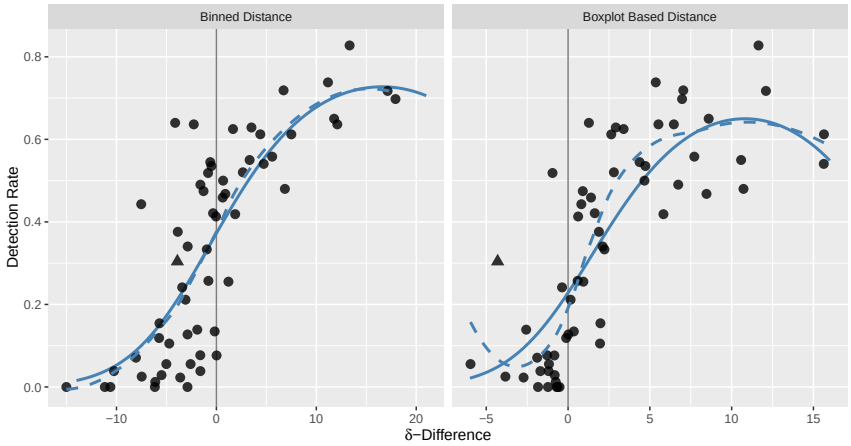
Figure 8b shows the relationship between detection rate and the γ-number of extreme null plots. As this number increases, it gets harder for subjects to identify the data plot. It is interesting to see that for some lineups subjects are able to pick the data plot even if there are one or two more extreme null plots.

Though distance based on boxplots works better a bit better, binned distance does a decent job in this case. According to the binned distance, there are a few lineups, in which the data plot is identified in more than 60% of all evaluations despite a negative δ-difference (see also Figure 8). It should be noted that the binned distance does not take any graphical elements of the plot (such as the box or whiskers) into account but calculates distance solely based on the data. So outliers may have an effect on the binned distance but might not affect the distance based on the boxplots.

If participants base their choice on graphical elements, binned distance might therefore not be able to adequately reflect this. In order to investigate on what participants base their choice, we are going to have a closer look at an individual lineup.

From Figure 8 we see that for some of the lineups the detection rate is higher than its δ-difference would suggest. One such lineup is marked using a triangle in Figure 8. Figure 9 shows the lineup and the distribution of distance metrics for a closer look at what might observers lead to pick the data plot as different. The grey numbers at the bottom right

(a) Scatterplots of detection rate versus δ-difference



(b) Scatterplots of detection rate versus γ-number of extreme nulls

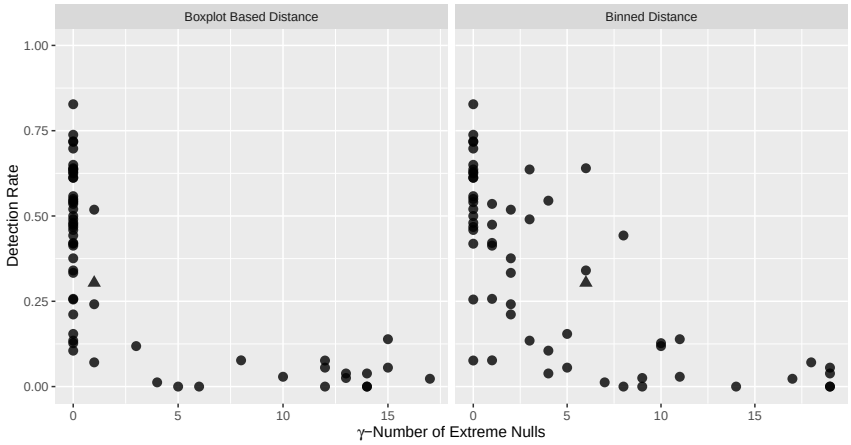


Figure 8: Comparison of distance metrics for side-by-side boxplots. Detection Rate (a) and the number of plots greater than the observed (b) are plotted against the difference based on the boxplot and binned distance. The vertical line represents the difference equal to zero when there is at least one null plot similar to the observed plot. The detection rate increases with the difference. As the number of plots with distance greater than the observed increases, the detection rate decreases. The triangle represents a lineup which has a high detection rate but a negative δ-difference. This particular lineup is examined in Figure 9.

of each of the plots in the lineup shows a summary of how often a plot was picked by a participant in 168 evaluations.

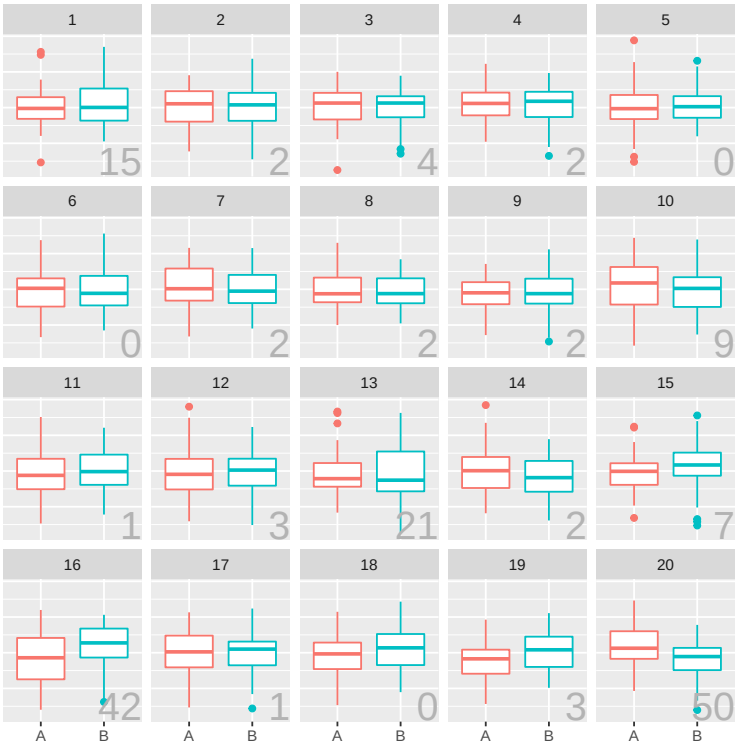
The observed data plot is Plot #20, which has been picked most often by participants, but there are other plots that are being chosen quite frequently. Plot #16 is the plot with the largest boxplot distance. This is reflected by the large number of times this plot has been singled out by observers.

Maybe surprisingly, plots Plots #19 and #15, which have relatively large differences between the quartiles, are not being chosen by many participants. Instead, observers seem to focus on the difference in interquartile ranges (i.e. the height of the box in a boxplot). Plots #1, #13 and #16 exhibit a large interquartile difference and are being picked often by observers.

The time subjects take to respond to a lineup is another measure that can be used to evaluate their difficulty. Due to the presence of some huge outliers, we decided to use the median of time taken for each lineup. These values are plotted against δ-difference for both distance measures as shown in Figure 10. Both δ-difference exhibit a similar pattern: the time to respond peaks at a δ-difference of zero. This indicates, that the situation where two or more plots exhibits similarly extreme features is the most difficult for observers to judge. With negative δ-differences at least one null plot is more extreme, and observers seem to be able to make their choice quickly (probably for the extreme null plot). When δ-difference is positive, the median time to respond decreases rapidly as δ-difference increases. Hence, subjects are able to make their choice of a plot more quickly if the true plot is extreme compared to the null plots.

Note that taking the log of time to respond is an alternative to using the median. Qualitatively, the relationships to distance metrics are very similar for median and log time taken, but median time is much easier to interpret.

(a) Lineup of side-by-side boxplots. The numbers at the bottom right are the number of times each of the plots was chosen by an observer.



(b) Boxplot based distance (c) Binned (2,8) distance (d) Binned (2,2) distance

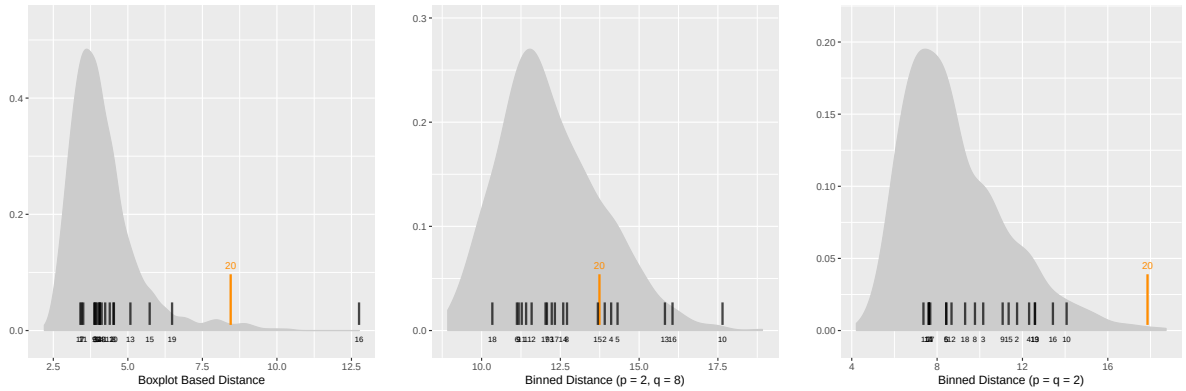


Figure 9: Illustration of the behavior of the three distance metrics. The lineup is shown in (a) and distributions of the different metrics based on this lineup is shown in the other plots: boxplot based distance in (b), binned distance with 2 and 8 bins on x and y axis in (c) and binned distance with 2 bins along both axes in (d). The lineup corresponds to the point marked with a triangle in difference vs. detection rate plot in Figure 8.

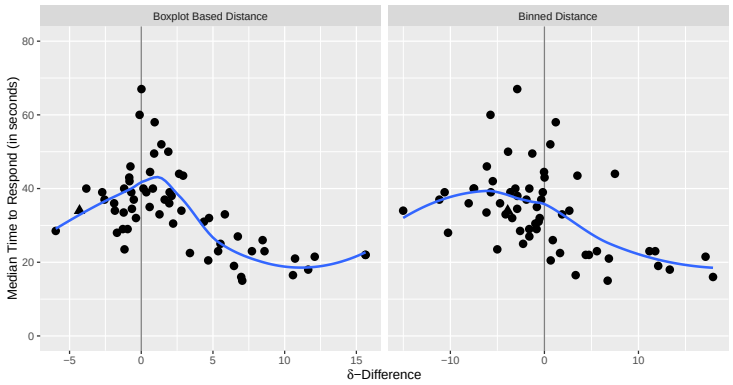


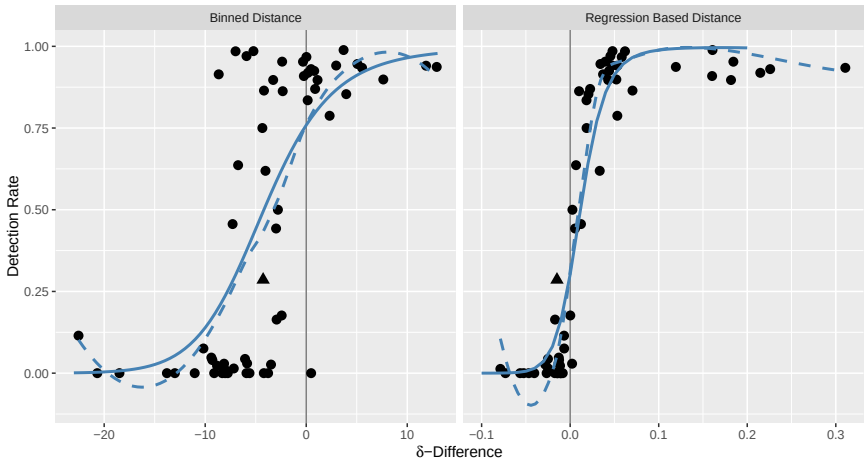
Figure 10: Comparison of distance metrics for side-by-side boxplots. Median time to respond is plotted against δ-difference based on boxplot and binned(2,8) distance. The vertical line represents a δ-difference equal to zero when there is at least one null plot similar to the observed plot. Median time to respond decreases as δ-difference increases. The triangle marks again the lineup examined in detail in Figure 9.

3.2 Experiment II – Scatterplots with an Overlaid Regression Line

The question of interest of experiment II is very similar to the one in experiment I: again, the focus is to investigate the power of visual methods in the framework of normal models. In contrast to experiment I, we are interested in the significance of a continuous variable X. The test statistic therefore is a scatterplot of the dependent variable and X overlaid by a regression line. As mentioned in the introduction and further discussed in section 5.2 of Majumder et al. (2013), X is assumed to be standard normal, and dependent data Y is also simulated from a normal distribution for various correlation settings. Null data correspondingly is simulated from $N(X\widehat{\beta}, \widehat{\sigma}^2)$. Figures 1 and 5 show examples of the type of lineup used in the study. Subjects recruited from MTurk were shown a set of ten lineups and asked to identify the plot with the steepest slope in each.

For each lineup in this experiment, distances between the plots were computed using both regression based distance (d_{RG}) and binned distances (d_{BN}) with a small number of bins. For each lineup the proportion of data identifications was calculated from participants' responses and plotted against δ-difference and the γ-number of extreme null plots, as shown in Figure 11.

(a) δ-difference



(b) γ-number of extreme nulls

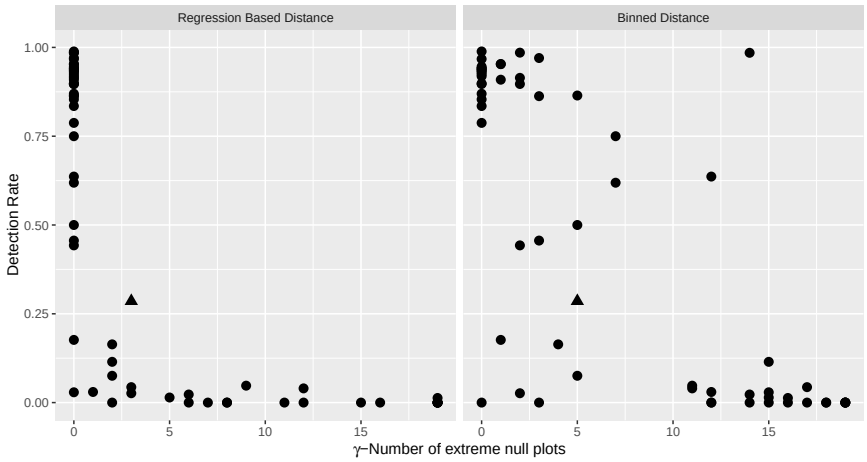


Figure 11: Comparison of distance metrics for scatterplots with a regression line overlaid. Detection rate is plotted against (a) δ-difference and (b) γ-number of extreme null plots based on regression and binned distances. The vertical line represents the difference equal to zero when there is at least one null plot with an identical difference measure to the data plot. Detection rate increases on average with δ-difference. As the γ-number of extreme null plots increases, detection rate decreases. The triangle represents a lineup which has high detection rate but negative difference. This particular lineup is examined in Figure 13.

As δ-difference increases, average detection rate increases, i.e. subjects do better in easier lineups than hard ones. The solid lines show fits of logistic regressions of detection rate in δ-difference based on regression (AIC: 746.9) and based on binned distance (AIC: 2150.7). Both fits come reasonably close to the dashed lines of a non-parametric loess smooth, indicating that they explain most of the relationship between δ-difference and detection rate. The regression based distance works well in capturing the complexity of the lineups. A few lineups have a δ-difference close to zero, marked by the vertical line – for those lineups detection rates of lineups flip from being close to zero to close to one within a very short interval.

For binned distance the situation is quite different. Although detection rate increases with difference, the detection rate is already quite high for lineups with negative differences. This is a classic scenario where the distance does not capture all the features on which observers base their choice: here, a graphical element –the line– affects the response, and shifts detection rates horizontally. While this makes an absolute comparison of distances across different types of plots impossible, we can still use binned distance as a relative measure to judge difficulty.

Figure 11b shows detection rate against the γ-number of extreme null plots. As the number of extreme plots increases, detection rate decreases on average — indicating that identifying the data plot from a lineup becomes harder when there are more extreme plots in the lineup. For a few lineups, almost all evaluations led to an identification of the data plot although there was one null plot with an extreme feature. From Figure 11a, we see that this difference is marginal in most cases, though.

Figure 12 shows the relationship between the median time taken to respond and δ-difference for both the distances. It can be clearly seen that there is a strong negative association: as δ-difference increases, the subjects take less time to respond. Similar to the previous example of section 3.1 time to respond peaks at a δ-difference close to zero.

Although the regression based distance seems to efficiently identify the quality of the lineup, there is one lineup (marked by a solid triangle in Figure 11) with a negative δ-difference which was nevertheless identified by observers reasonably successfully. Figure 13 shows the lineup and the corresponding distributions of distance metrics.

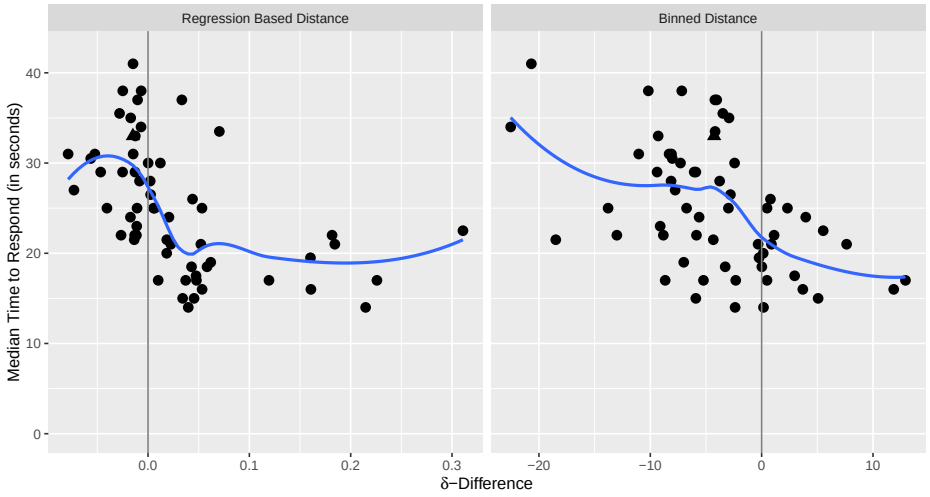


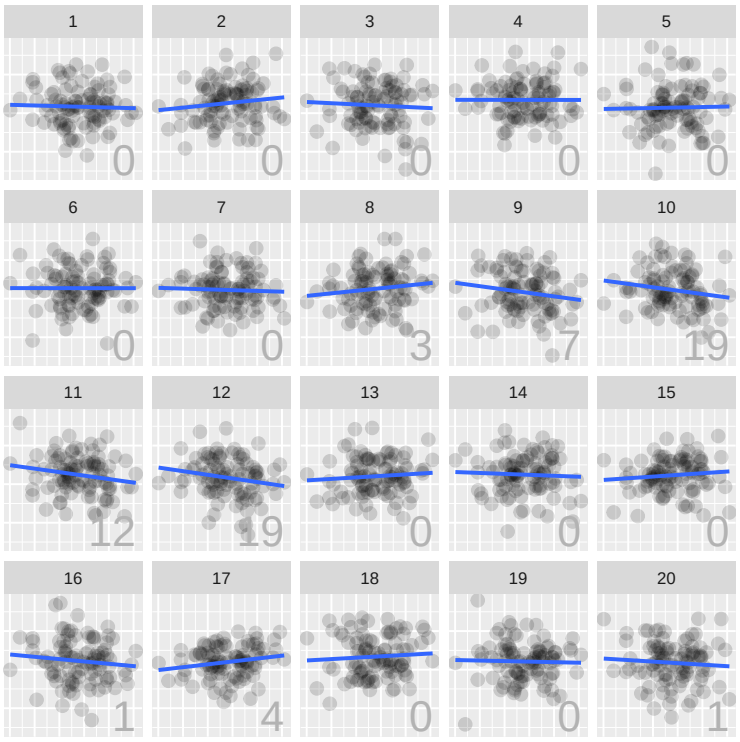
Figure 12: Comparison of distance metrics for scatterplots with a regression line over laid. Median time to respond is plotted against δ-difference based on regression based and binned(2,2) distance. The vertical line represents a δ-difference equal to zero, i.e. there is at least one null plot similar to the observed plot. The median time to response decreases as δ-difference increases. The triangle represents a lineup which is examined in Figure 13.

The lineup in Figure 13 is a difficult one as suggested by the distribution of the distance metrics based on regression. For the data plot (in panel #10) the conventional p-value for testing the slope equal to zero is 0.085. However, the signal in the plot is strong enough, to make around 28% of all subjects pick this plot.

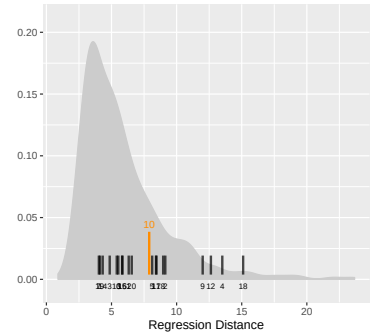
The binned distance with 2 bins on each axes does not let the data plot stand out in any way, however, the binned distance using the optimal number of bins (8 on the x-axis and 2 on the y-axis) by the optimal number of bins selection method identifies the data plot as different from the others.

The number of picks lines up best with the difference measure based on the slope (regression without intercept). Plots #10, 12, 11, 9, and 7 all have a relatively steep slope, and are also the plots that were picked the most often. Again, a distance measure derived directly from one of the graphical elements in the plot leads to the best assessment of the choices made by human evaluators.

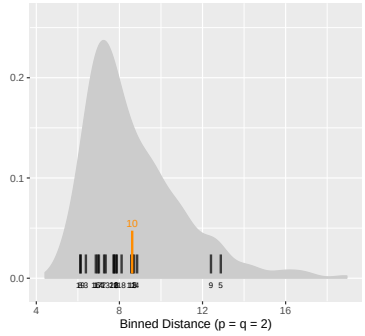
(a) Lineup of scatterplots with overlaid regression lines. The numbers at the bottom right of each panel gives the number of times this plot was chosen in 66 evaluations.



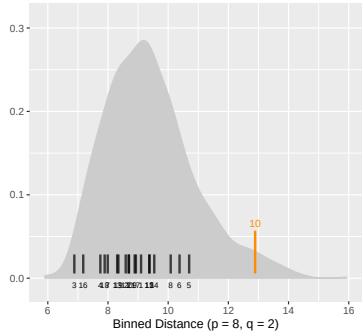
(b) Regression based distance



(c) Binned (2,2) distance



(d) Binned (8,2) distance



(e) p-values

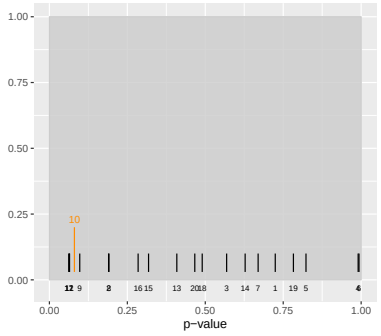


Figure 13: Illustration of the behavior of different distance metrics. The lineup is shown in (a) and the distributions of different distance metrics using this lineup are shown in plots (b)–(d): regression based distances in (b), binned distance with 2 bins on each axes in (c), and binned distance with 8 and 2 bins in x and y axis (d). In (e), the distribution of the conventional p-values are plotted with p-values for the lineups marked on the distribution. The lineup corresponds to the point marked with a triangle in difference vs. detection rate plot in Figure 11.

3.3 Experiment III – Large p, Small n Data

The motivation behind this experiment is to study the effect of high dimensions on separability in data. Scenarios with pure noise and some real separation in two or three groups were investigated. A projection pursuit with Penalized Discriminant Analysis Index (Lee and Cook, 2010) was used to obtain one (for two groups) or two (for three groups) dimensional projections. Depending on the number of groups, either a jittered dotplot or a scatterplot was used as test statistic in a lineup setting. The null plots are obtained by permuting the group variable and plotting the two dimensional projections obtained from a projection pursuit with PDA index. The subjects were shown these lineups and were asked to identify the plot with the most separated colored groups. Figure 14 gives an example of such a lineup of a two dimensional projection with three colored groups.

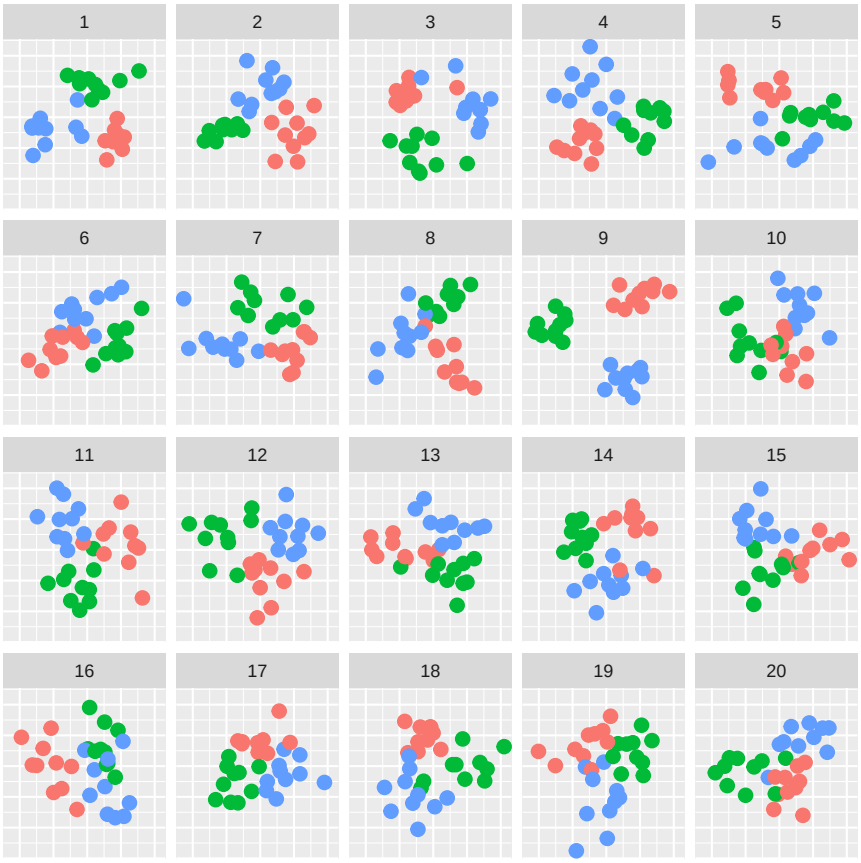
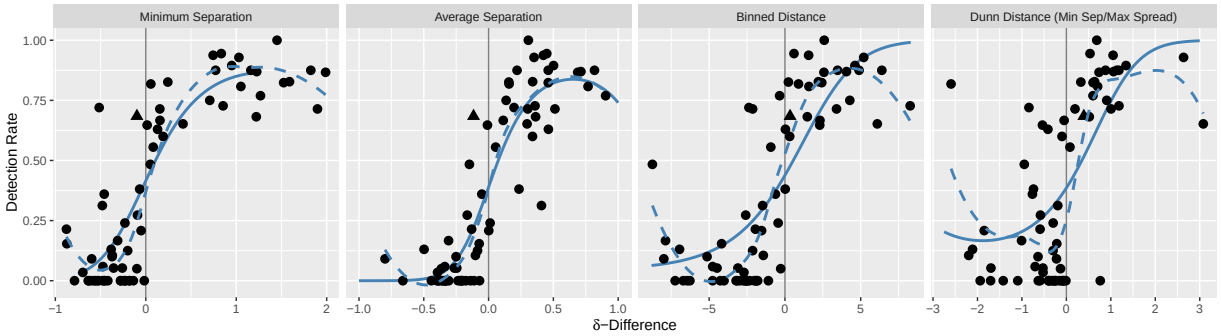


Figure 14: An example lineup from Experiment III. Here, two dimensional projections of the PDA index are plotted for $n = 30$ observations in 20 dimensional data with separation. The subjects were asked to identify the plot with the most separated colors. Can you identify the data plot?

The distances between the plots in this experiment were computed using the distance based on minimum separation and average separation of the clusters and also the binned distance. The number of bins used for the lineups with one dimensional projections is larger (10 in this case) but for the lineups with two dimensional projections, the number of bins used is 5. The proportion of correct response is plotted against δ-difference and γ-number of extreme nulls for both distances. Figure 15 shows the results.

(a) δ-difference



(b) γ-number of extreme null plots

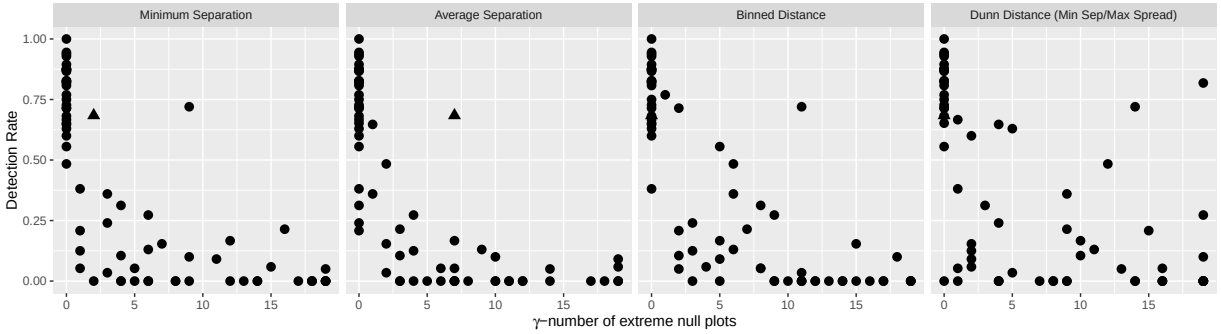


Figure 15: Comparison of distance metrics for the scatterplot with clusters. Detection rate is plotted against (a) δ-difference and (b) against γ-number of extreme nulls, using distances based on minimum separation, average separation, binned and Dunn's distance. The vertical line represents the difference equal to zero when there is at least one null plot similar to the observed plot. Solid blue line represents the fitted logistic regression model and the dashed blue line shows a loess smoother. Detection rate generally increases with δ-difference. As the γ-number of extreme null plots increases, detection rate decreases. The triangle represents a lineup with high detection rate and negative difference based on the average separation distance. This is examined in Figure 17.

In Figure 15, the detection rate is plotted against the difference for distance based on minimum separation, average separation and the binned distance. The vertical line shows a difference equal to zero. It can be seen that as the difference increases, the detection rate increases and all distances do a reasonably good job in capturing the response of the subjects. In terms of the logistic regression fit to the data, average separation is a bit ahead according to AIC (AIC: 349.6) compared to minimal separation (AIC: 422.8) and binned distance (AIC: 543.4). Dunn separation, motivated from cognitive perception, comes in at a maybe surprising last place (AIC: 697.3).

In (b) it can be seen that as there are more extreme null plots compared to the observed plot, the subjects find it difficult to pick the observed plot. For a few lineups, a large number of the subjects identify the observed plot although there is more extreme null plots.

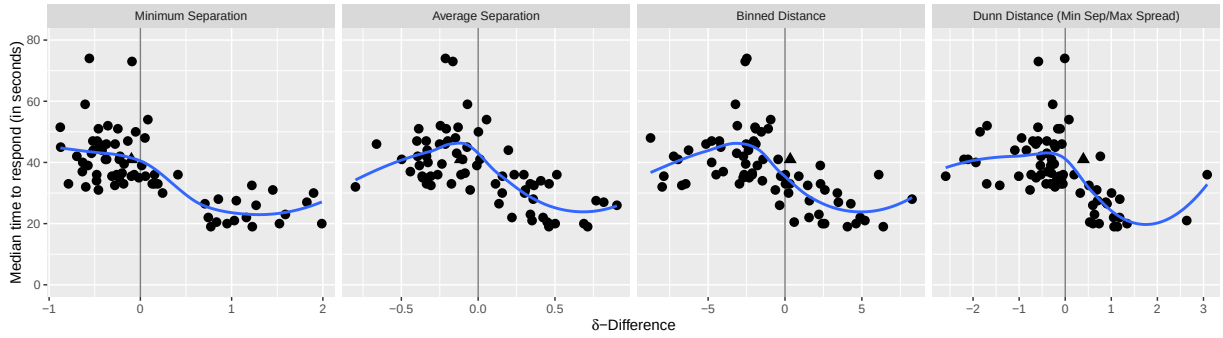
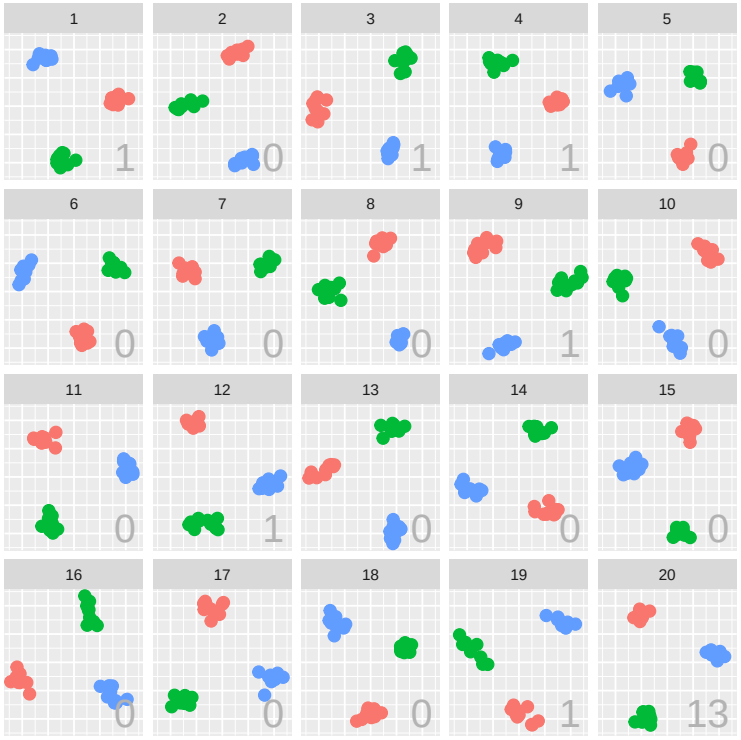


Figure 16: Plot showing the median time to respond by the subjects against the difference based on the minimum separation distance, average separation and binned distance. The vertical line represents the difference equal to 0 when there is at least one null plot similar to the observed plot. The median time decreases as the difference increases.

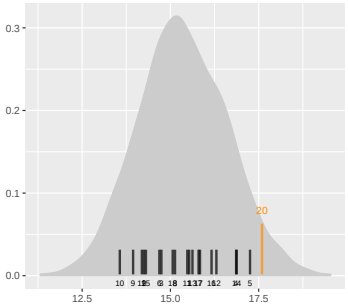
Figure 16 shows the relationship between the median time observers take to respond and δ-difference for the three different distances. It can be clearly seen that there is a strong negative association; as the difference increases, subjects take less time to respond. For both average separation and binned distance we see a peak in response time, i.e. for large negative δ-difference the median time to respond decreases again.

Figure 17 shows the lineup in a high dimension, low sample size setting. The number of dimensions used is 100 and two of the dimensions have some separation. Plot #20 shows the two-dimensional projections of the original data. This plot is, indeed, chosen in 13 out of 19 evaluations. As the true plot does have real separation, it is to be expected

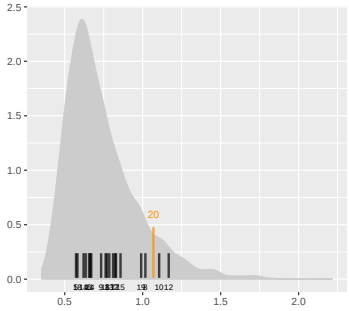
(a) Lineup of scatterplots of three groups. Which plot shows the best separation?



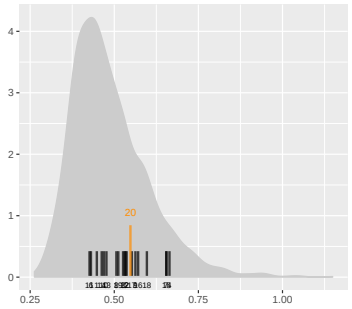
(b) Binned (5,5) Distance



(c) Minimum Separation



(d) Average Separation



(e) Dunn Separation

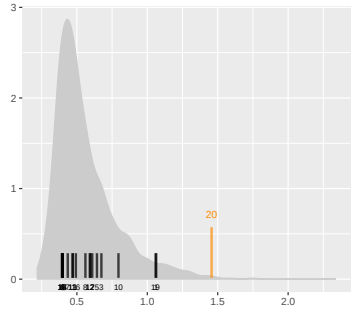


Figure 17: Illustration of the behavior of different distance metrics. The lineup is shown in (a) and the distributions of different distance metrics are shown in the other plots: binned distance with 6 and 4 bins in x and y axis respectively in (b), distance based on minimum separation in (c), distance based on average separation in (d) and distance based on Dunn separation in (e). The reference distributions are based on 100 null sets of 19 nulls each, yielding 1,800 distances.

that subjects would be able to identify the plot. The distance based on average separation yields a negative difference showing that the lineup is difficult, while the distance based on minimum separation yields a positive difference. The distance metrics identify different characteristics in a plot. The average separation looks at the average of the distances of the points in a cluster to the points in other clusters. Dunn separation performs very well in this example and correctly identifies the data panel as the panel with the strongest signal. While the binned distance shows plot #20 as the one with the largest distance, this should be taken with care, because binned distance is, unlike the other two distances, not rotation invariant. In the case of plot #20 the large distance merely indicates the difference in the arrangement of the clusters rather than their separation.

4 Conclusion

Distance metrics are compared to the response of human subjects on lineups. While there is a fairly strong amount of agreement in most situations, in some situations they disagree. There does not seem to be one single reason behind this disagreement. Observers might identify a plot as different from the others in a lineup because of multiple features. However, distance metrics are constructed such that they take one specific property of a plot into account.

Distance metrics can be used to automatically and objectively assess the difficulty of a lineup before showing the lineups to human subjects. Hence, they allow us to provide lineups within a range of difficulty to human subjects to evaluate.

In classical inference, the test statistic follows a certain distribution under the null hypothesis. Similarly, null plots in visual inference can be viewed as random samples from the null distribution. Though theoretically this is true, practically it is impossible to exhaustively investigate such a distribution. The distribution of the distance metrics approximates one dimension of the null distribution for a given distance metric. The value of the distance metric for the actual plot can be compared to all the other plots using such a distribution.

The reason of choice can provide a way of evaluating the performance of a distance metric. For example, if the reason of choice for a majority of observers is the steepest slope,

for a lineup of scatterplots with regression line overlaid, the regression based distance may work better than the binned distance. Similarly, if the reason of choice is the presence of outliers, the binned distance with large number of bins on both axes may be the best distance metric to reflect detection rates.

What we see in each of the experiments is that the general approach of the binned distance, while mostly performing decently, is out-done by a distance that is more tailored to the question of interest or takes the graphical elements into account. This is only to be expected. What the lineup protocol opens up to us is an approach that delivers us some objective insight into what people respond to in a plot and which graphical elements they consider when viewing a plot.

Acknowledgement: All plots are done with the `ggplot2` (Wickham, 2009) package in R. The document is written in `knitr` (Xie, 2015).

SUPPLEMENTARY MATERIAL

Software: R-package `nullabor` containing code to create lineups and calculate the distance measures described in the article. Available on CRAN (R Development Core Team, 2015), with development versions at https://github.com/dicook/nullabor.

Reproducibility: All the code and anonymized data used in this analysis is available at https://github.com/niladrir/metrics-paper.

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Appendix

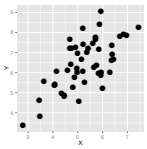
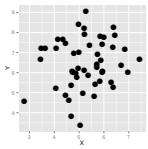
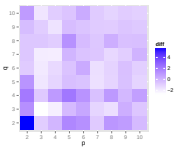
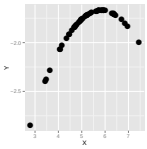
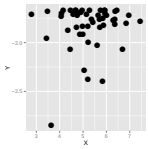
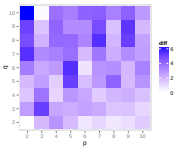
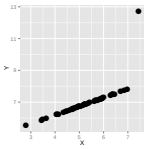
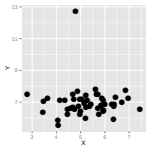
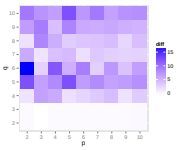
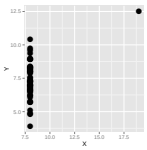
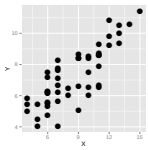
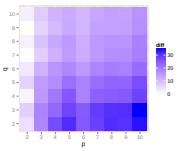
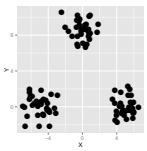
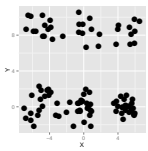
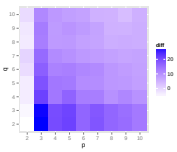
Effect of the Number of Bins on Distance

Binned distance works for any type of data and for any null generating mechanism. It is based on the raw data but does not take into account the graphical elements in the plot. Binned distance can be used in situations where no distance measure is known for the particular plot type and hence it can be regarded as universal. But the the number of bin highly affect the distance. An unfortunate choice may lead to hard to interpret or conflicting results.

We investigate the choice of the number of bins using different types of data and different null generating mechanisms. Null datasets are obtained for a true data set using a null generating mechanism and hence a lineup is constructed. As described in section sec:dists mean binned distances are calculated between the true data and the null datasets and also among the null datasets. The number of bins for the binned distance are varied from 2 to 10 on both x and y direction and δ-difference is determined for each combination. Tables 2

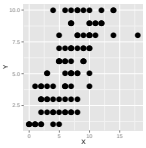
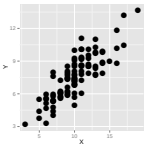
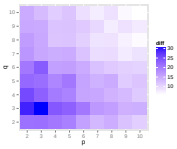
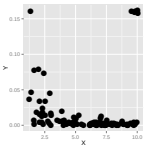
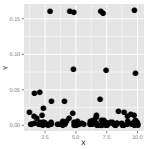
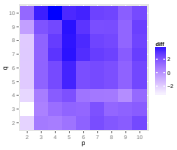
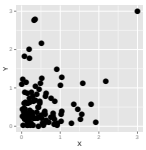
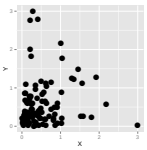
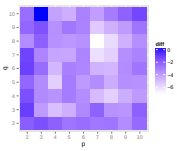
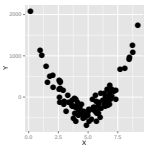
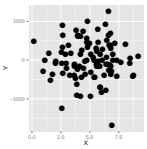
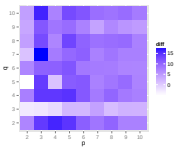
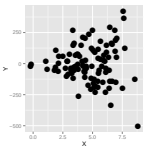
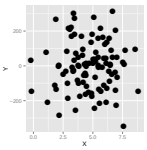
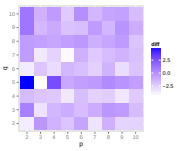
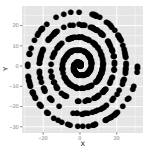
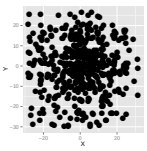
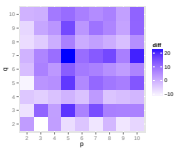
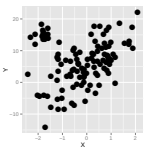
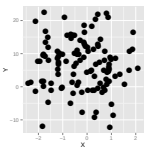
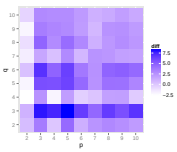
and 3 show the type of data, the observed plot, the null generating mechanism (NGM), a typical null plot, δ-difference and the maximally observed value of δ, together with the corresponding number of bins in x and y direction. Similarly, the minimal δ value and its parameters are collected to get an idea of the range of values.

Table 2: Preferable number of bins for different types of observed data to calculate the binned distance.

Data	Observed Plot	NGM	Typical Null	Difference	(x-bin, y-bin) Min, Max
Linear association		Permutation			(2,2) -2.5, 5.7
Nonlinear relationship		Permutation			(2,10) 0.0, 6.2
Linear with outliers		Permutation			(2,6) -0.4, 16.7
Same x with one outlier		Simulation from Poi(9)			(10, 3) -0.1, 34.3
Clusters		Permutation			(3,2) -5.7, 37.6

The rationale behind selecting different types of data is to investigate how the optimal number of bins or bin sizes varies with different types of data. The different null generating mechanisms are also selected for the same reason. In Table 2 the first four observed data plots corresponds in spirit to the datasets described by Francis Anscombe (Anscombe, 1972), using a larger number of data points. The fifth dataset is a data set with 3 distinct clusters. In Table 3, the first dataset shows a categorical dataset. The second and the third data are non-linear association and skewed with the presence of outliers. The fourth and fifth datasets are residual plots with a curved pattern and non-constant variance pattern.

Table 3: Preferable number of bins for different types of observed data to calculate the binned distance.

Data	Observed Plot	NGM	Typical Null	Difference	(x-bin, y-bin) Min, Max
Categorical		Simulation from $N(\mu, \sigma^2)$			(3,3) 6.2, 30.7
Nonlinear with outliers		Permutation			(4, 10) -3.4, 3.9
Skewed with outliers		Permutation			(3,10) -7.1, 0.3
Residual		Simulation from null model			(3,7) -4.5, 17.8
Residual		Simulation from null model			(2,5) -4.4, 4.8
Spiral		Permutation			(5,7) -11.9, 23.6
Contaminat		Permutation			(5,3) -2.5, 8.1

The sixth data is a spiral data while the seventh one is a data with contamination.

The δ-differences are represented in a tile plot where each tile gives the difference for each combination. Darker hues correspond to larger differences values. It can be seen that these tile plots look different for the different datasets. Hence the optimal number of bins varies from data to data. No specific pattern is evident in the plot. But overall it can be seen that for strong linear relationships, small number of bins should be preferred over large number of bins. Also when outliers are present in the data, larger number of bins are preferred on at least one of the axes.

It is important to mention at this point that Tables 2 and 3 is not meant to provide any guidelines for the selection of number of bins. The Tables only show that binned distance is highly affected by the number of bins and the type of data. It is advisable to find the optimal number of bins for a given dataset before using binned distance.