HistogramTools for Distributions of Large Data Sets

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Abstract

Histograms are a common graphical representation of the distribution of a data set. They are particularly useful for collecting very large data sets into a binned form for easier data storage and analysis. The **HistogramTools** R package augments the built-in support for histograms with a number of methods that are useful for analyzing large data sets. Specifically, methods are included for serializing histograms into a compact Protocol Buffer representation for sharing between distributed tasks, functions for manipulating the resulting aggregate histograms, and functions for measuring and visualizing the information loss associated with histogram representations of a data set.

1 Introduction

Histograms have been used for over a century (Pearson 1895) as a compact graphical representation of a distribution of data. Support for generating histograms is included in almost all statistical software, including R. However, the growth in large-scale data analysis in R with the MapReduce (Dean and Ghemawat 2008) paradigm has highlighted the need for some extensions to the histogram functionality in R(R Core Team 2012) for the collection, transmission, and manipulation of larged binned data sets.

Much previous work on histograms (Sturges 1926; Scott 1979) involves identifying ideal breakpoints for visualizing a data set. Our context is different; we use histograms as compact representations in a large MapReduce environment, and need to merge histograms from subsets of the data to obtain a histogram for the whole data set. In this case, the challenges are engineering challenges, rather than visualization challenges. For example, how do we efficiently store large numbers of histograms generated frequently by real-time monitoring systems of many thousands of computers? How can we aggregate histograms generated by different tasks in a large scale computation? If we chose very granular bucket boundaries for our initial data collection pass, how can we then reshape the bucket boundaries to be more relevant to the analysis questions at hand?

2 Parallel Data Collection Patterns

Many large data sets in fields such as particle physics and information processing are stored in binned or histogram form in order to reduce the data storage requirements (Scott 2009).

There are two common patterns for generating histograms of large data sets with MapReduce. In the first method, each mapper task can generate a histogram over a subset of the data that is has been assigned, and then the histograms of each mapper are sent to one or more reducer tasks to merge.

In the second method, each mapper rounds a data point to a bucket width and outputs that bucket as a key and '1' as a value. Reducers then sum up all of the values with the same key and output to a data store.

In both methods, the mapper tasks must choose identical bucket boundaries even though they are analyzing disjoint parts of the input set that may cover different ranges, or we must implement multiple phases.
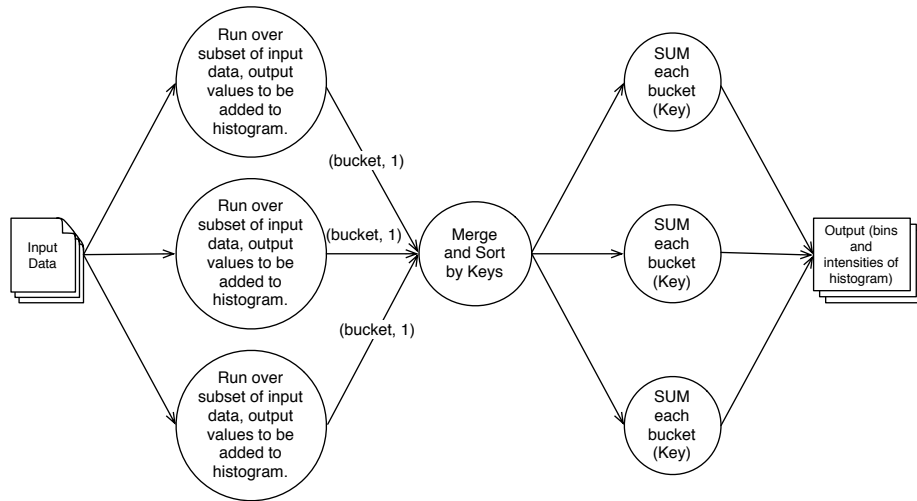

Figure 1: Diagram of MapReduce Histogram Generation Pattern

Figure 1 illustrates the second method described above for histogram generation of large data sets with MapReduce.

This package is designed to be helpful if some of the Map or Reduce tasks are written in R, or if those components are written in other languages and only the resulting output histograms need to be manipulated in R.

3   Efficient Representations of Histograms

Consider an example histogram of 100 random data points. Figure 2 shows the graphical representation and list structure of R histogram objects.

```
> myhist <- hist(runif(100))
```

This histogram compactly represents the full distribution. Histogram objects in R are lists with 6 components: breaks, counts, density, mids, name, and equidist.

If we are working in a parallel environment and need to distribute such a histogram to other tasks running in a compute cluster, we need to serialize this histogram object to a binary format that can be transferred over the network.

3.1   Native R Serialization

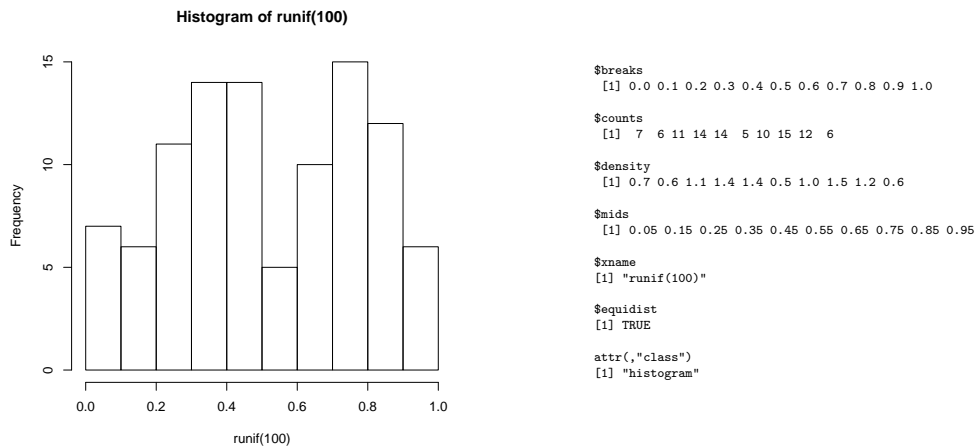R includes a built-in serialization framework that allows one to serialize any R object to an Rdata file.

Histogram of runif(100)

```
$breaks
 [1] 0.0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1.0

$counts
 [1]  7  6 11 14 14  5 10 15 12  6

$density
 [1] 0.7 0.6 1.1 1.4 1.4 0.5 1.0 1.5 1.2 0.6

$mids
 [1] 0.05 0.15 0.25 0.35 0.45 0.55 0.65 0.75 0.85 0.95

$xname
[1] "runif(100)"

$equidist
[1] TRUE

attr(,"class")
[1] "histogram"
```

Figure 2: Example Histogram

```
> length(serialize(myhist, NULL))
```

```
[1] 543
```

This works and is quite convenient if the histogram must only be shared between tasks running the R interpreter, but it is not a very portable format.

3.2 Protocol Buffers

Protocol Buffers are a flexible, efficient, automated, cross-platform mechanism for serializing structured data (Pike, Dorward, Griesemer, and Quinlan 2005; Google 2012). The RProtoBuf package (Francois, Eddelbuettel, and Stokely 2012) provides an interface for manipulating protocol buffer objects directly within R.

Of the 6 elements stored in an R histogram object, we only need to store three in our serialization format since the others can be re-computed. This leads to the following simple protocol buffer definition of the breaks, counts, and name of a histogram:

```
package HistogramTools;

 message HistogramState {
   repeated double breaks = 1;
   repeated int32 counts = 2;
   optional string name = 3;
 }
```

The package provides `as.Message` and `as.histogram` methods for converting between R histogram objects and this protocol buffer representation.

In addition to the added portability, the protocol buffer representation is significantly more compact.

```
> hist.msg <- as.Message(myhist)
```

Our histogram protocol buffer has a human-readable ASCII representation:

3

```
> cat(as.character(hist.msg))

breaks: 0
breaks: 0.1
breaks: 0.2
breaks: 0.30000000000000004
breaks: 0.4
breaks: 0.5
breaks: 0.60000000000000009
breaks: 0.70000000000000007
breaks: 0.8
breaks: 0.9
breaks: 1
counts: 7
counts: 6
counts: 11
counts: 14
counts: 14
counts: 5
counts: 10
counts: 15
counts: 12
counts: 6
name: "runif(100)"
```

But it is most useful when serialized to a compact binary representation:

```
> length(hist.msg$serialize(NULL))
```

```
[1] 131
```

This protocol buffer representation is not compressed by default, however, so we can do better:

```
> raw.bytes <- memCompress(hist.msg$serialize(NULL), "gzip")
> length(raw.bytes)
```

```
[1] 90
```

We can then send this compressed binary representation of the histogram over a network or store it to a cross-platform data store for later analysis by other tools. To recreate the original R histogram object from the serialized protocol buffer we can use the `as.histogram` method.

```
> uncompressed.bytes <- memDecompress(raw.bytes, "gzip")
> new.hist.proto <- P("HistogramTools.HistogramState")$read(uncompressed.bytes)
> length(uncompressed.bytes)
```
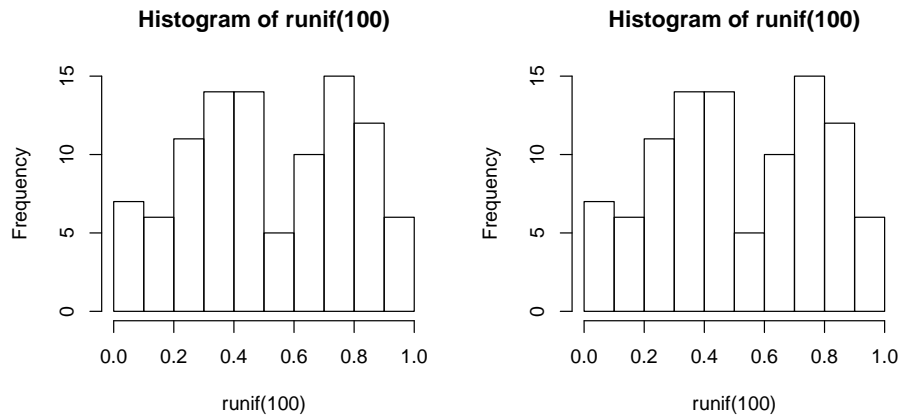
```
[1] 131
```

The resulting histogram is the same as the original; it was converted to a protocol buffer, serialized, compressed, then uncompressed, parsed, and converted back to a histogram.

```
> plot(myhist)
> plot(as.histogram(new.hist.proto))
```

4 Quantiles and Cumulative Distribution Functions

When histograms are used as a binned data storage mechanism to reduce data storage cost, information about the underlying distribution is lost. We can however approximate the quantiles and cumulative distribution function for the underying distribution from the histogram.

The `Count`, `ApproxMean`, and `ApproxQuantile` functions are meant to help with this, but note that they will only be accurate with very granular histogram buckets. They would rarely be appropriate with histogram buckets chosen by the default algorithm in R.

```
> hist <- hist(c(1,2,3), breaks=c(0,1,2,3,4,5,6,7,8,9), plot=FALSE)

> Count(hist)

[1] 3

> ApproxMean(hist)

[1] 1.5

> ApproxQuantile(hist, .5)

50%
1.5

> ApproxQuantile(hist, c(.05, .95))

 5% 95%
0.6 5.1
```

The `HistToEcdf` function takes a histogram and returns an empirical distribution function similar to what is returned by the `ecdf` function on a distribution.

```
> h <- hist(runif(100), plot=FALSE)
> e <- HistToEcdf(h)
> e(.5)

[1] 0.46
```

```
> par(mfrow=c(1,2))
> plot(h)
> plot(HistToEcdf(h))
> par(mfrow=c(1,1))
```
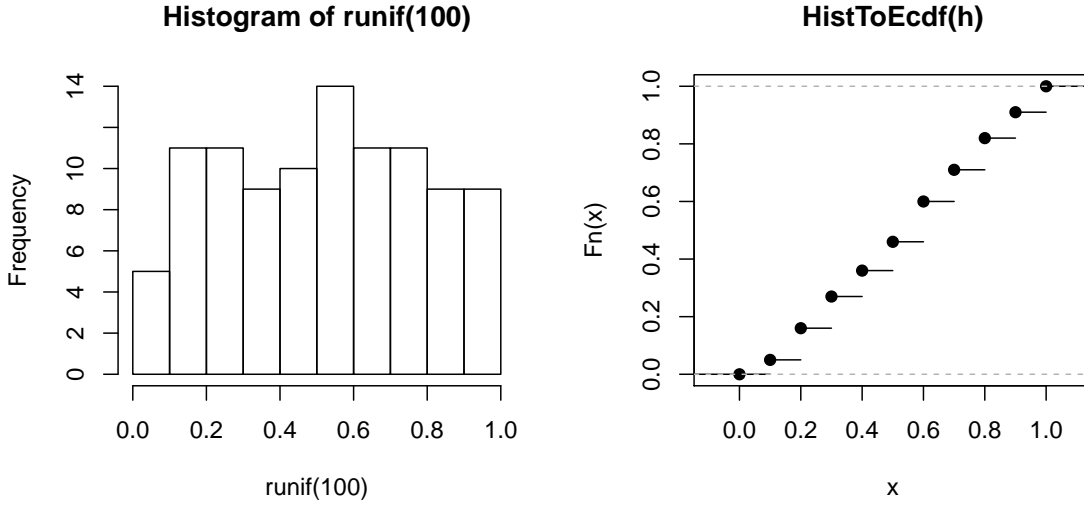

Figure 3: Histogram and CDF Created with HistToEcdf

5   Error estimates in CDFs approximated from histograms

When constructing cumulative distribution functions from binned histogram data sets there will usually be some amount of information loss. We can however come up with an upper bound for the error by looking at two extreme cases. For a given histogram h with bucket counts C_i for $1 \leq i \leq n$ and left-closed bucket boundaries B_i for $1 \leq i \leq n+1$, we construct two data sets. Let X be the (unknown) underlying data set for which we now only have the binned representation h. Let $X_{\min}$ be the data set constructed by assuming the data points in each bucket of the histogram are all equal to the left bucket boundary. Let $X_{\max}$ be the data set constructed by assuming the data points in each bucket of the histogram are at the right bucket boundary. Then F_X is the true empirical CDF of the underlying data, and $F_{X_{\min}}(x) \geq F_X(x) \geq F_{X_{\max}}(x)$.

$$X_{\min} = \left((B_i)_{k=1}^{C_i} : 1 \leq i \leq n \right) X_{\max} = \left((B_{i+1})_{k=1}^{C_i} : 1 \leq i \leq n \right)$$

The package provides two different distance metrics to measure the difference between empirical cumulative distribution functions $F_{X_{\min}}$ and $F_{X_{\max}}$. These distances serve as upper-bounds for the amount of error between the true empirical distribution function F_X of the unbinned data and an ECDF calculated from the binned data.

5.1 Kolmogorov-Smirnov Distance of the Cumulative Curves

The first metric provided by the package is the two-sample Kolmogorov-Smirnov distance between $X_{\min}$ and $X_{\max}$. In other words, it the largest possible distance between cumulative distribution functions that could be represented by the binned data. This metric is more formally defined as

$$\sup_x |F_{X_{\max}}(x) - F_{X_{\min}}(x)|$$

This function is also occasionally called the maximum displacement of the cumulative curves (MDCC).

```
> x <- rexp(1000)
> h <- hist(x, breaks=c(0,1,2,3,4,8,16,32), plot=FALSE)
> x.min <- rep(head(h$breaks, -1), h$counts)
> x.max <- rep(tail(h$breaks, -1), h$counts)
> ks.test(x.min, x.max, exact=F)

        Two-sample Kolmogorov-Smirnov test

data:  x.min and x.max
D = 0.608, p-value < 2.2e-16
alternative hypothesis: two-sided

> KSDCC(h)

[1] 0.608
```

The `KSDCC` function accepts a histogram, generates the largest and smallest empirical cumulative distribution functions that could be represented by that histogram, and then calculates the Kolmogorov-Smirnov distance between the two CDFs. This measure can be used in cases where expanding the binned data into `x.min` and `x.max` explicitly to calculate distances using e.g. `ks.test` directly would not be feasible. Figure 4 illustrates geometrically what value is being returned.

5.2 Earth Mover's Distance of the Cumulative Curves

The "Earth Mover's Distance" is like the Kolmogorov-Smirnof statistic, but uses an integral to capture the difference across all points of the curve rather than just the maximum difference. This is also known as Mallows distance, or Wasserstein distance with $p = 1$.

The value of this metric for our histogram h is

$$\int_{\mathbb{R}} |F_{X_{\max}}(x) - F_{X_{\min}}(x)| dx,$$

Figure 5 shows the same e.c.d.f of the binned data represented in the previous section, but with the yellow boxes representing the range of possible values for any real e.c.d.f. having the same binned representation. For any distribution X with the binned representation in h, the e.c.d.f $F(X)$ will pass only through the yellow boxes. The area of the yellow boxes is the Earth Mover's Distance.

```
> x <- rexp(100)
> h1 <- hist(x, plot=FALSE)
> h2 <- hist(x, breaks=seq(0,round(max(x) + 1),by=0.1), plot=FALSE)
> KSDCC(h1)

[1] 0.34
```
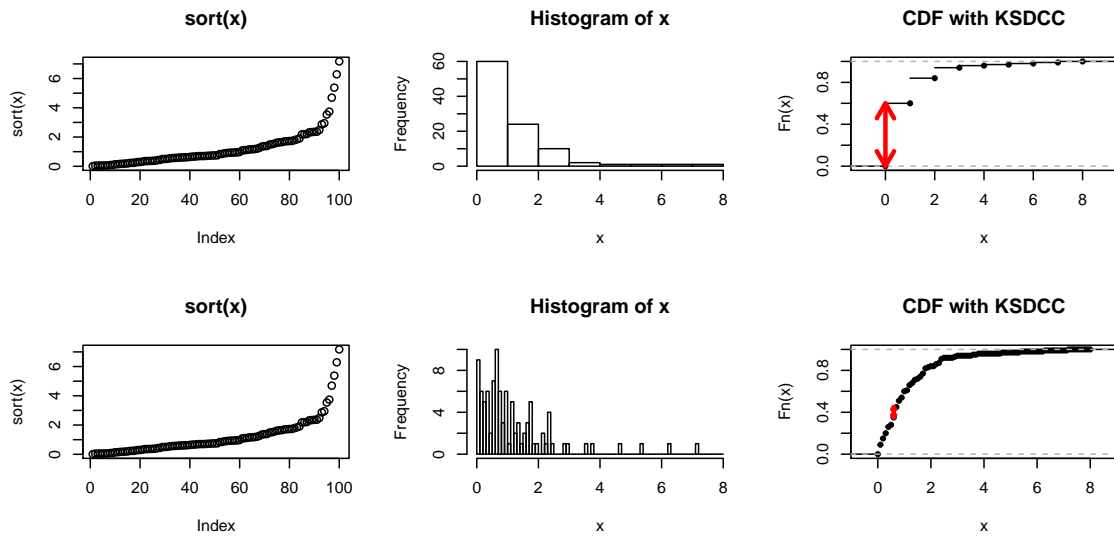
Figure 4: Sorted raw data (column 1), Histograms (column 2), CDF with KSDCC (column 3)
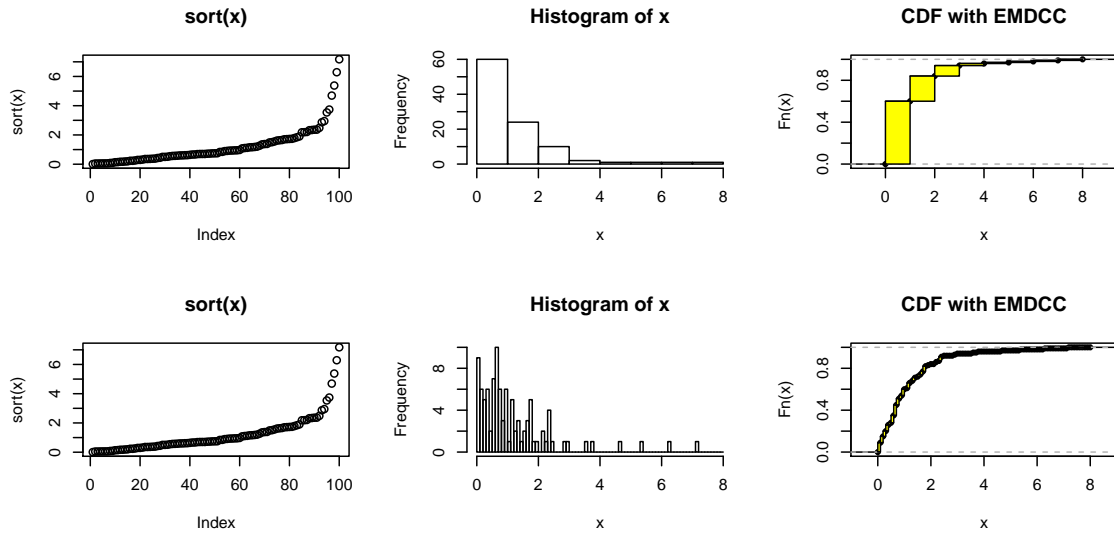

Figure 5: Sorted raw data (column 1), Histograms (column 2), CDF with EMDCC (column 3)

```
> KSDCC(h2)
[1] 0.12
```

```
> EMDCC(h1)

[1] 0.1

> EMDCC(h2)

[1] 0.01666667
```

So, using this metric, the second lower example with more granular histogram bins produces an ECDF with reduced worst case error bounds compared to the one with default buckets, as expected.

6 Histogram Bin Manipulation

6.1 Trimming Empty Buckets from the Tails

When generating histograms with a large number of fine-grained bucket boundaries, the resulting histograms may have a large number of empty consecutive buckets on the left or right side of the histogram. The `TrimHistogram` function can be used to remove them as illustrated in Figure 6.

```
> hist.1 <- hist(runif(100,min=2,max=4), breaks=seq(0,6,by=.2), plot=FALSE)
> hist.trimmed <- TrimHistogram(hist.1)

> length(hist.1$counts)

[1] 30

> sum(hist.1$counts)

[1] 100

> length(hist.trimmed$counts)

[1] 10

> sum(hist.trimmed$counts)

[1] 100

> par(mfrow=c(1,2))
> plot(hist.1)
> plot(TrimHistogram(hist.1), main="Trimmed Histogram")
```

6.2 Adding/Merging Histograms

If histograms (for different data sets) have the same bucket boundaries, it is possible to add them together to obtain the histogram for the combined data set by aggregating the counts values with the `AddHistograms` function illustrated in Figure 7.

```
> hist.1 <- hist(c(1,2,3,4), plot=FALSE)
> hist.2 <- hist(c(1,2,2,4), plot=FALSE)
> hist.sum <- AddHistograms(hist.1, hist.2)
```

`AddHistograms` accepts an arbitrary number of histogram objects to aggregate as long as they have the same bucket boundaries.

Figure 6: Effect of the `TrimHistogram` function.

Figure 7: Effect of the `AddHistograms` function.

```
>    hist.1 <- hist(c(1,2,3), breaks=0:9, plot=FALSE)
>    hist.2 <- hist(c(1,2,3), breaks=0:9, plot=FALSE)
>    hist.3 <- hist(c(4,5,6), breaks=0:9, plot=FALSE)
>    hist.sum <- AddHistograms(hist.1, hist.2, hist.3)
>    hist.sum

$breaks
 [1] 0 1 2 3 4 5 6 7 8 9

$counts
```
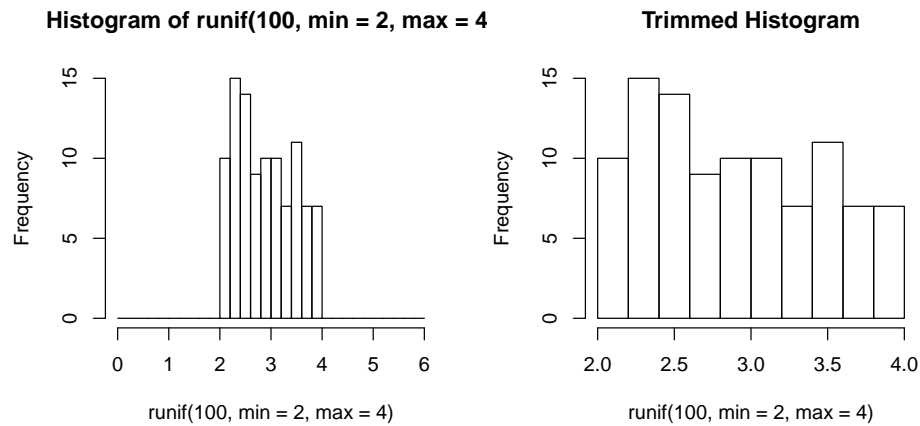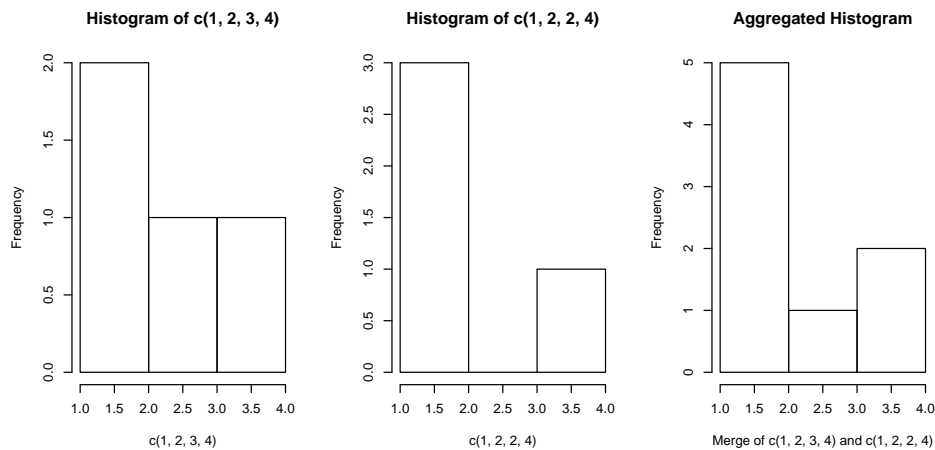
```
[1] 2 2 2 1 1 1 0 0 0

$density
[1] 0.2222222 0.2222222 0.2222222 0.1111111 0.1111111 0.1111111
[7] 0.0000000 0.0000000 0.0000000

$mids
[1] 0.5 1.5 2.5 3.5 4.5 5.5 6.5 7.5 8.5

$xname
[1] "Merge of 3 histograms"

$equidist
[1] TRUE

attr(,"class")
[1] "histogram"
```

6.3 Merging Buckets

We may want a version of a histogram with fewer buckets, to save storage or to produce better plots. The MergeBuckets function takes a histogram and a parameter for the number of adjacent buckets to merge together and returns a new histogram with different bucket boundaries as illustrated in Figure 8.

```
> overbinned <- hist(c(rexp(100), 1+rexp(100)), breaks=seq(0, 10, by=.01), plot=FALSE)
> better.hist <- MergeBuckets(overbinned, adj=30)
```
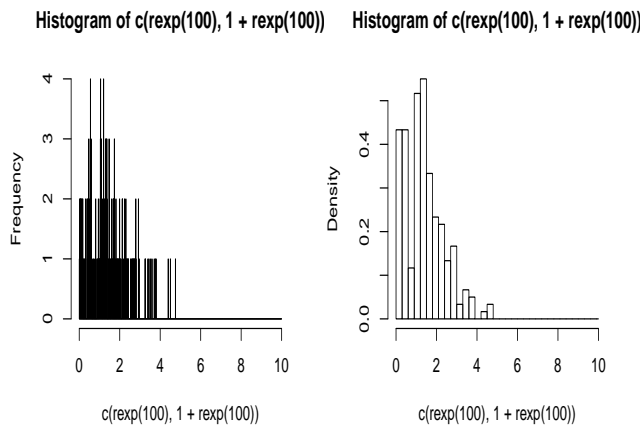

Figure 8: Effect of the MergeBuckets function.

6.4 Subsetting Histograms

The `SubsetHistogram` function takes a histogram and a new minimum and maximum bucket boundary and returns a new histogram with a subset of the buckets as illustrated in Figure 9.

```
> hist.1 <- hist(runif(100, min=0, max=10), breaks=seq(from=0, to=10, by=.5), plot=FALSE)
> hist.2 <- SubsetHistogram(hist.1, minbreak=2, maxbreak=6)
```
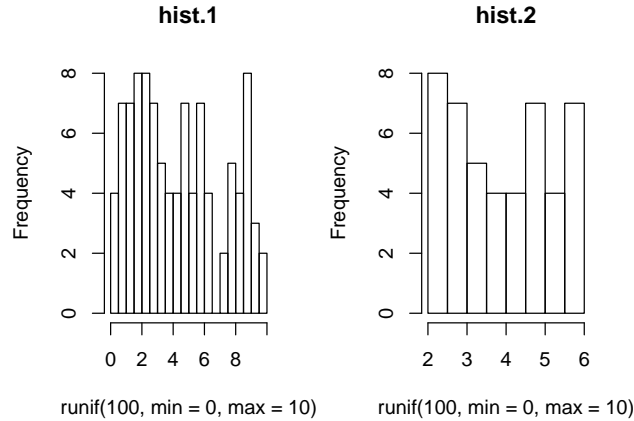

Figure 9: Effect of the `SubsetHistogram` function.

7 Histogram Distance Measures

This package provides a number of metrics for computing a distance measure for two histograms. At the moment, only bin-by-bin similarity measures are supported meaning that the two histograms must have exactly the same bucket boundaries. The attributes of the different distance measures are described in (Rubner, Tomasi, and Guibas 2000).

7.1 Minkowski Distance

The Minkowski distance of order p between two histograms can be computed with the `minkowski.dist` function.

```
> h1 <- hist(runif(100), plot=FALSE)
> h2 <- hist(runif(100), plot=FALSE)
> minkowski.dist(h1, h2, 1)

[1] 54

> minkowski.dist(h1, h2, 2)

[1] 21.9545

> minkowski.dist(h1, h2, 3)
```

```
[1] 17.11115

> # Verify the implementation:
> p <- 3
> #dist(t(matrix(c(h1$counts, h2$counts), nrow=2)), "minkowski", p=p)
> # Or, alternatively:
> (sum(abs(h1$counts - h2$counts)^p))^(1/p)

[1] 17.11115
```

7.2   Histogram Intersection Distance

The histogram intersection distance (Swain and Ballard 1991) between two histograms can be computed with the `intersect.dist` function.

```
> intersect.dist(h1, h2)

[1] 0.27
```

7.3   Kullback-Leibler Divergence

The Kullback-Leibler Divergence (Kullback 1997) between two histograms can be computed with the `kl.divergence` function.

```
> kl.divergence(h1, h2)

[1] 27.47632
```

7.4   Jeffrey Divergence

The `jeffrey.divergence` function computes the Jeffrey divergence between two histograms (Puzicha, Hofmann, and Buhmann 1997).

```
> jeffrey.divergence(h1, h2)

[1] 14.74318
```

# 8   Visualization

8.1   Average Shifted Histograms

Average shifted histograms are a simple device for taking a collection of m histograms each with uniform bin width h, but with bin origins offset/shifted (Scott 2009).

Given the focus of this package on large data sets, a HistToASH function is provided to produce the average shifted histogram from a single histogram assuming the underlying dataset is no longer available in unbinned form. The next plot shows the original density histogram of the overlaid with the average shifted histogram with smoothing parameter 5.

```
> x <- runif(1000, min=0, max=100)
> h <- hist(x, breaks=0:100, plot=F)
> plot(h,freq=FALSE, main="Histogram of x with ASH superimposed in red")
> # Superimpose the Average Shifted Histogram on top of the original.
> lines(HistToASH(h), col="red")

[1] "ash estimate nonzero outside interval ab"
```

Histogram of x with ASH superimposed in red
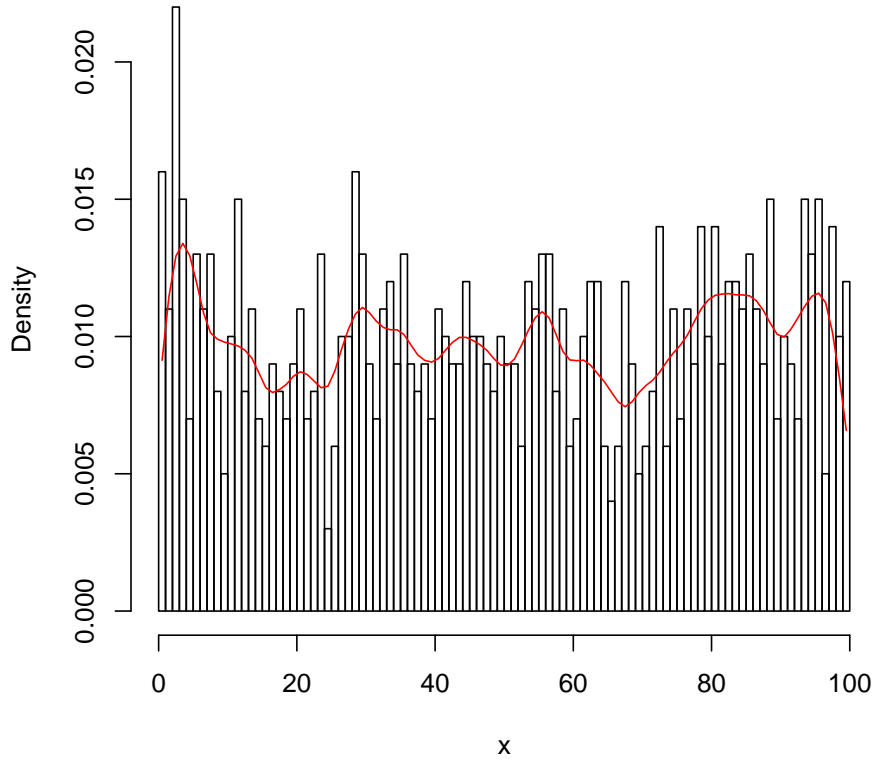
8.2 Log-scale Histograms

Many histograms encountered in databases, distributed systems, and other areas of computer science use log-scaled bucket boundaries and may still contain counts that vary exponentially.

Examples of such data sets include the size or age of files stored, or the latency enountered by read requests. Such histograms can be read into R using the methods of this package, but the default plotting functionality is not very useful.

For example, Figure 10 shows the default plot output for the histogram of read sizes observed when building a FreeBSD kernel. Neither the density histogram (left) nor the frequency histogram (middle) make it easy to understand the distribution. In contract, the log ECDF produced by the `PlotLog2ByteEcdf` function makes it easy to see that about 20% of the reads were of 64 bytes or smaller, and that the median read size was well under a kilobyte.

9 Summary

The HistogramTools package presented in this paper has been in wide use for the last several years to allow engineers to read distribution data from internal data stores written in other languages.
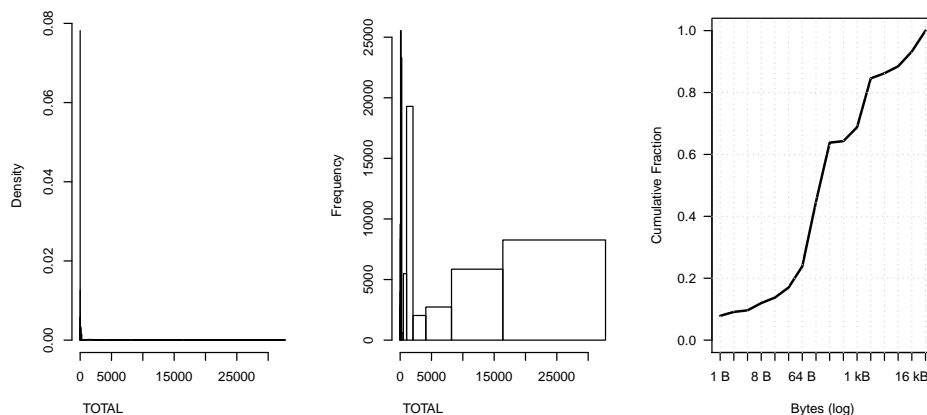
Figure 10: Example Log Log Histogram Data

Internal production monitoring tools and databases, as well as the output of many MapReduce jobs have been used.

References

Dean J, Ghemawat S (2008). "MapReduce: simplified data processing on large clusters." *Communications of the ACM*, **51**(1), 107–113.

Francois R, Eddelbuettel D, Stokely M (2012). *RProtoBuf: R Interface to the Protocol Buffers API*. R package version 0.2.6, URL `http://cran.r-project.org/web/packages/RProtoBuf/index.html`.

Google (2012). *Protocol Buffers: Developer Guide*. URL `http://code.google.com/apis/protocolbuffers/docs/overview.html`.

Kullback S (1997). *Information theory and statistics*. Courier Dover Publications.

Pearson K (1895). "Contributions to the mathematical theory of evolution. II. Skew variation in homogeneous material." *Philosophical Transactions of the Royal Society of London. A*, **186**, 343–414.

Pike R, Dorward S, Griesemer R, Quinlan S (2005). "Interpreting the data: Parallel analysis with Sawzall." *Sci. Program.*, **13**(4), 277–298. ISSN 1058-9244.

Puzicha J, Hofmann T, Buhmann JM (1997). "Non-parametric similarity measures for unsupervised texture segmentation and image retrieval." In *Computer Vision and Pattern Recognition, 1997. Proceedings., 1997 IEEE Computer Society Conference on*, pp. 267–272. IEEE.

R Core Team (2012). *R: A Language and Environment for Statistical Computing*. R Foundation for Statistical Computing, Vienna, Austria. ISBN 3-900051-07-0, URL `http://www.R-project.org/`.

Rubner Y, Tomasi C, Guibas LJ (2000). "The earth mover's distance as a metric for image retrieval." *International Journal of Computer Vision*, **40**(2), 99–121.

Scott DW (1979). "On optimal and data-based histograms." *Biometrika*, **66**(3), 605–610.

Scott DW (2009). *Multivariate density estimation: theory, practice, and visualization*, volume 383. Wiley. com.

Sturges HA (1926). "The choice of a class interval." *Journal of the American Statistical Association*, **21**(153), 65–66.

Swain MJ, Ballard DH (1991). "Color indexing." *International journal of computer vision*, **7**(1), 11–32.