Scalable and Numerically Stable Descriptive Statistics in SystemML

Yuanyuan Tian   Shirish Tatikonda   Berthold Reinwald

IBM Almaden Research Center, USA

{ytian, statiko, reinwald}@us.ibm.com

Abstract—**With the exponential growth in the amount of data that is being generated in recent years, there is a pressing need for applying machine learning algorithms to large data sets. SystemML is a framework that employs a declarative approach for large scale data analytics. In SystemML, machine learning algorithms are expressed as scripts in a high-level language, called DML, which is syntactically similar to R. DML scripts are compiled, optimized, and executed in the SystemML runtime that is built on top of MapReduce.**

As the basis of virtually every quantitative analysis, *descriptive statistics* provide powerful tools to explore data in SystemML. In this paper, we describe our experience in implementing descriptive statistics in SystemML. In particular, we elaborate on how to overcome the two major challenges: (1) achieving numerical stability while operating on large data sets in a distributed setting of MapReduce; and (2) designing scalable algorithms to compute order statistics in MapReduce. By empirically comparing to algorithms commonly used in existing tools and systems, we demonstrate the numerical accuracy achieved by SystemML. We also highlight the valuable lessons we have learned in this exercise.

I. Introduction

The growing need to analyze massive data sets has led to an increased interest in implementing machine learning algorithms on MapReduce [9], [11]. SystemML [10] is an Apache Hadoop based system for large scale machine learning, developed at IBM Research. In SystemML, machine learning algorithms are expressed as scripts written in a high-level language, called DML, with linear algebra and mathematical primitives. SystemML compiles these scripts, applies various optimizations based on data and system characteristics, and translates them into efficient runtime on MapReduce. A wide variety of machine learning techniques can be expressed in SystemML, including classification, clustering, regression, matrix factorization, and ranking.

Besides complex machine learning algorithms, SystemML also provides powerful constructs to compute *descriptive statistics*. Descriptive statistics primarily include *univariate analysis* that deals with a single variable at a time, and *bivariate analysis* that examines the degree of association between two variables. Table I lists the descriptive statistics that are currently supported in SystemML. In this paper, we describe our experience in addressing the two major challenges when implementing descriptive statistics in SystemML – (1) numerical stability while operating on large data sets in the distributed setting of MapReduce; (2) efficient implementation of order statistics in MapReduce.

TABLE I
Descriptive statistics supported in SystemML

Univariate	**Scale variable:** Sum, Mean, Harmonic mean, Geometric mean, Min, Max, Range, Median, Quantiles, Inter-quartile mean, Variance, Standard deviation, Coefficient of variation, Central moment, Skewness, Kurtosis, Standard error of mean, Standard error of skewness, Standard error of kurtosis **Categorical variable:** Mode, Per-category frequencies
Bivariate	**Scale-Scale variables:** Covariance, Pearson correlation **Scale-Categorical variables:** Eta, ANOVA F measure **Categorical-Categorical variables:** Chi-squared coefficient, Cramer's V, Spearman correlation

Most of descriptive statistics, except for order statistics, can be expressed in certain summation form, and hence it may seem as if they are trivial to implement on MapReduce. However, straightforward implementations often lead to disasters in numerical accuracy, due to overflow, underflow and round-off errors associated with finite precision arithmetic. Such errors often get magnified with the increasing volumes of data that is being processed. However in practice, the issue of numerical stability is largely ignored, especially in the context of large scale data processing. Several well-known and commonly used software products still use numerically unstable implementations to compute several basic statistics. For example, McCullough and Heiser highlighted in a series of articles that Microsoft Excel suffers from numerical inaccuracies for various statistical procedures [15], [16], [17], [18]. In their studies, they conducted various tests related to univariate statistics, regression, and Monte Carlo simulations using the NIST Statistical Reference Datasets (StRD) [3]. They note that numerical improvements were made to univariate statistics only in the recent versions of Excel [15]. In the context of large-scale data processing, Hadoop-based systems such as PIG [19] and HIVE [20] still use numerically unstable implementations to compute several statistics. PIG as of version 0.9.1 supports only the very basic *sum* and *mean* functions, and neither of them use numerically stable algorithms. The recent version of HIVE (0.7.1) supports more statistics including *sum*, *mean*, *variance*, *standard deviation*, *covariance*, and *Pearson correlation*. While *variance*, *standard deviation*, *covariance*, and *Pearson correlation* are computed using stable methods, both *sum* and *mean* are computed using numerically unstable methods. These examples highlight the fact that the issue of numeric stability has largely been ignored in practice, in spite of its utmost importance.

In this paper, we share our experience in achieving numerical stability as well as scalability for descriptive statistics on MapReduce, and bring the community's attention to the important issue of numerical stability for large scale data processing. Through a detailed set of experiments, we demonstrate the scalability and numerical accuracy achieved by SystemML. We finally conclude by highlighting the lessons we have learned in this exercise.

II. Numerical Stability

Numerical stability refers to the inaccuracies in computation resulting from finite precision floating point arithmetic on digital computers with round-off and truncation errors. Multiple algebraically equivalent formulations of the same numerical calculation often produce very different results. While some methods magnify these errors, others are more robust or stable. The exact nature and the magnitude of these errors depend on several different factors like the number of bits used to represent floating point numbers in the underlying architecture (commonly known as *precision*), the type of computation that is being performed, and also on the number of times a particular operation is performed. Such round-off and truncation errors typically grow with the input data size. Given the exponential growth in the amount of data that is being collected and processed in recent years, numerical stability becomes an important issue for many practical applications.

One possible strategy to alleviate these errors is to use special software packages that can represent floating point values with *arbitrary* precision. For example, $BigDecimal$ in Java provides the capability to represent and operate on arbitrary-precision signed decimal numbers. Each $BigDecimal$ number is a Java object. While the operations like addition and subtraction on native data types (double, int) are performed on hardware, the operations on $BigDecimal$ are implemented in software. Furthermore, JVM has to explicitly manage the memory occupied by $BigDecimal$ objects. Therefore, these software packages often suffer from significant performance overhead. In our benchmark studies, we observed up to 2 orders of magnitude slowdown for addition, subtraction, and multiplication using $BigDecimal$ with precision 1000 compared to the native $double$ data type; and up to 5 orders of magnitude slowdown for division.

In the rest of this section, we discuss methods adopted in SystemML to calculate descriptive statistics, which are both numerically stable and computationally efficient. We will also highlight the common pitfalls that must be avoided in practice. First, we discuss the fundamental operations *summation* and *mean*, and subsequently present the methods that we use for computing *higher-order statistics* and *covariance*.

A. Stable Summation

Summation is a fundamental operation in many statistical functions, such as mean, variance, and norms. The simplest method is to perform *naive recursive summation*, which initializes $sum = 0$ and incrementally updates sum. It however suffers from numerical inaccuracies even on a single computer. For instance, with 2-digit precision, naive summation of numbers $1.0, 0.04, 0.04, 0.04, 0.04, 0.04$ results in 1.0, whereas the exact answer is 1.2. This is because once the first element 1.0 is added to sum, adding 0.04 will have no effect on sum due to round-off error. A simple alternative strategy is to first sort the data in increasing order, and subsequently perform the naive recursive summation. While it produces the accurate result for the above example, it is only applicable for non-negative numbers, and more importantly, it requires an expensive sort.

There exists a number of other methods for stable summation [12]. One notable technique is proposed by Kahan [13]. It is a *compensated summation* technique – see Algorithm 1. This method maintains a *correction* or *compensation* term to accumulate errors encountered in naive recursive summation.

Algorithm 1 Kahan Summation Incremental Update

```
// $s_1$ and $s_2$ are partial sums, $c_1$ and $c_2$ are correction terms
KahanIncrement($s_1, c_1, s_2, c_2$){
  $corrected\_s_2 = s_2 + (c_1 + c_2)$
  $sum = s_1 + corrected\_s_2$
  $correction = corrected\_s_2 - (sum - s_1)$
  return $(sum, correction)$ }
```

Kahan and Knuth independently proved that Algorithm 1 has the following relative error bound [12]:

$$\frac{|E_n|}{|S_n|} = \frac{|\hat{S}_n - S_n|}{|S_n|} \leq (2u + O(nu^2))\kappa_X, \tag{1}$$

where $S_n = \sum_{i=1}^{n} x_i$ denotes the true sum of a set of n numbers $X = \{x_1, x_2, ..., x_n\}$, and $\hat{S}_n$ is the sum produced by the summation algorithm, $u = \frac{1}{2}\beta^{1-t}$ is the *unit roundoff* for a floating point system with base β and precision t. It denotes the upper bound on the relative error due to rounding. For IEEE 754 floating point standard with $\beta = 2$ and $t = 53$, $u = 2^{-53} \approx 10^{-16}$. Finally, κ_X is known as the *condition number* for the summation problem, and it is defined as the fraction $\frac{\sum_{i=1}^{n} |x_i|}{|\sum_{i=1}^{n} x_i|}$. The condition number measures the sensitivity of the problem to approximation errors, independent of the exact algorithm used. Higher the value of κ_X, the higher will be the numerical inaccuracies and the relative error. It can be shown that for a random set of numbers with a nonzero mean, the condition number of summation asymptotically approaches to a finite constant as $n \to \infty$. Evidently, the condition number is equal to 1 when all the input values are non-negative. It can be seen from Equation 1 that when $nu \leq 1$, the bound on the relative error is independent of input size n. In the context of IEEE 754 standard, it means that when n is in the order of 10^{16} the relative error can be bounded independent of the problem size. In comparison, the naive recursive summation has a relative error bound $\frac{|E_n|}{|S_n|} \leq (n-1)u\kappa_X + \frac{O(u^2)}{|\sum_{i=1}^{n} x_i|}$ [12], which clearly is a much larger upper bound when compared to Equation 1.

One can easily extend the Kahan algorithm to the MapReduce setting. The resulting algorithm is a MapReduce job in which each mapper applies KAHANINCREMENT and generates a partial sum with correction, and a single reducer produces the final sum.

Through error analysis, we can derive the relative error bound for this MapReduce Kahan summation algorithm: $\frac{|E_n|}{|S_n|} \leq [4u+4u^2+O(mu^2)+O(\frac{n}{m}u^2)+O(mu^3)+O(\frac{n}{m}u^3)+O(nu^4)]\kappa_X$ (see Appendix for proof). Here, m is the number of mappers (m is at most in 1000s). As long as $\frac{n}{m}u \leq 1$ (and $m \ll n$), the relative error is independent of the number of input data items. In the context of IEEE 754 standard, it can be shown that when $\frac{n}{m}$ is in the order of $2^{53} \approx 10^{16}$, the relative error can be bounded independent of n. In other words, as long as the number of elements processed by each mapper is in the order of 10^{16}, the overall summation is robust with respect to the total number of data items to be summed. Therefore, by partitioning the work across multiple mappers, the MapReduce summation method is able to scale to larger data sets while keeping the upper bound on relative error independent of the input data size n.

B. Stable Mean

Mean is a fundamental operation for any quantitative data analysis. The widely used technique is to divde the sum by the total number of input elements. This straightforward method of computing mean however suffers from numerical instability. As the number of data points increases, the accuracy of sum decreases, thereby affecting the quality of mean. Even when the stable summation is used, sum divided by count technique often results in less accurate results.

In SystemML, we employ an incremental approach to compute the mean. This method maintains a running mean of the elements processed so far. It makes use of the update rule in Equation 2. In a MapReduce setting, all mappers apply this update rule to compute the partial values for count and mean. These partial values are then aggregated in the single reducer to produce the final value of mean.

$$n = n_a + n_b, \;\; \delta = \mu_b - \mu_a, \;\; \mu = \mu_a \oplus n_b \frac{\delta}{n} \tag{2}$$

In Equation 2, n_a and n_b denote the partial counts, μ_a and μ_b refer to partial means. The combined mean is denoted by μ, and it is computed using the KAHANINCREMENT function in Algorithm 1, denoted as $\oplus$ in the equation. In other words, we keep a correction term for the running mean, and $\mu = \mu_a \oplus n_b \frac{\delta}{n}$ is calculated via $(\mu.value, \mu.correction) =$ KAHANINCREMENT $(\mu_a.value, \mu_a.correction, n_b\frac{\delta}{n}, 0)$. Note that the use of KAHANINCREMENT is important to obtain stable value for μ. When the value of $n_b\frac{\delta}{n}$ is much smaller than μ_a, the resulting μ will incur a loss in accuracy – which can be alleviated by using KAHANINCREMENT. As we show later in Section IV, this incremental algorithm results in more accurate results. We also use it in stable algorithms to compute higher order statistics and covariance (see Sections II-C & II-D).

C. Stable Higher-Order Statistics

We now describe our stable algorithms to compute higher-order statistics, such as variance, skewness and kurtosis. The core computation is to calculate the p^{th} central moment $m_p = \frac{1}{n}\sum_{i=1}^{n}(x_i - \bar{x})^p$. Central moment can be used to describe higher-order statistics. For instance, variance $\sigma^2 = \frac{n}{n-1}m_2$, skewness $g_1 = \frac{m_3}{m_2^{1.5}} \cdot (\frac{n-1}{n})^{1.5}$, and kurtosis $g_2 = \frac{m_4}{m_2^2} \cdot (\frac{n-1}{n})^2 - 3$. The standard two-pass algorithm produces relatively stable results (for m_2, the relative error bound is $nu + n^2u^2\kappa_X^2$, where $\kappa_X = (\frac{\sum_{i=1}^{n} x_i^2}{\sum_{i=1}^{n}(x_i-\bar{x})^2})^{\frac{1}{2}}$ is the condition number), but it requires two scans of data – one scan to compute $\bar{x}$ and the second to compute m_p. A common technique (pitfall) is to apply a simple textbook rewrite to get a one-pass algorithm. For instance, m_2 can be rewritten as $\frac{1}{n}\sum_{i=1}^{n} x_i^2 - \frac{1}{n^2}(\sum_{i=1}^{n} x_i)^2$. The sum of squares and sum can be computed in a single pass. However, this algebraical rewrite is known to suffer from serious stability issues resulting from cancellation errors when performing subtraction of two large and nearly equal numbers (relative error bound is $nu\kappa_X^2$). This rewrite, as we show later in Section IV-B, may actually produce a negative result for m_2, thereby resulting in grossly erroneous values for variance and other higher-order statistics.

In SystemML, we use a stable MapReduce algorithm that is based on an existing technique [5], to incrementally compute central moments of arbitrary order. It makes use of an update rule (Equation 3) that combines partial results obtained from two disjoint subsets of data (denoted as subscripts a and b). Here, n, μ, M_p refer to the cardinality, mean, and $n \times m_p$ of a subset, respectively. Again, $\oplus$ represents addition through KAHANINCREMENT. When $p = 2$, the algorithm has a relative error bound of $nu\kappa_X$. While there is no formal proof to bound the relative error when $p > 2$, we empirically observed that this method produces reasonably stable results for skewness and kurtosis. In the MapReduce setting, the same update rule is used in each mapper to maintain running values for these variables, and to combine partial results in the reducer. Note that the update rule in [5] uses basic addition instead of the more stable KAHANINCREMENT. In Section IV-D, we will evaluate the effect of KAHANINCREMENT on the accuracy of higher-order statistics.

$$\begin{aligned} n &= n_a + n_b, \;\; \delta = \mu_b - \mu_a, \;\; \mu = \mu_a \oplus n_b \frac{\delta}{n} \\ M_p &= M_{p,a} \oplus M_{p,b} \oplus \{\sum_{j=1}^{p-2}\binom{p}{j}[(-\frac{n_b}{n})^j M_{p-j,a} \\ &\quad + (\frac{n_a}{n})^j M_{p-j,b}]\delta^j + (\frac{n_a n_b}{n}\delta)^p[\frac{1}{n_b^{p-1}} - (\frac{-1}{n_a})^{p-1}]\} \end{aligned} \tag{3}$$

D. Stable Covariance

Covariance $(\frac{\sum_{i=1}^{n}(x_i-\bar{x})(y_i-\bar{y})}{n-1})$ is one of the basic bivariate statistics. It measures the strength of correlation between two data sets. A common textbook one-pass technique rewrites the equation as $\frac{1}{n-1}\sum_{i=1}^{n} x_i y_i - \frac{1}{n(n-1)}\sum_{i=1}^{n} x_i \sum_{i=1}^{n} y_i$. Similar to the one-pass rewrite of variance described in Section II-C, this rewrite also suffers from numerical errors and can produce grossly inaccurate results.

In SystemML, we adapt the technique proposed by Bennett *et al.* [5] to the MapReduce setting. This algorithm computes the partial aggregates in the mappers and combines the partial aggregates in a single reducer. The update rule for computing $C = \sum_{i=1}^{n}(x_i - \bar{x})(y_i - \bar{y})$ is shown below. Note that $\oplus$ represents addition through KAHANINCREMENT. The difference between the update rule used in SystemML and the original update rule in [5] is that SystemML uses KAHANINCREMENT for the updates instead of the basic addition. In Section IV-D, we will empirically compare these two methods.

$$\begin{aligned} n &= n_a + n_b, \quad \delta_x = \mu_{x,b} - \mu_{x,a}, \quad \mu_x = \mu_{x,a} \oplus n_b \frac{\delta_x}{n} \\ \delta_y &= \mu_{y,b} - \mu_{y,a}, \quad \mu_y = \mu_{y,a} \oplus n_b \frac{\delta_y}{n} \\ C &= C_a \oplus C_b \oplus \frac{n_a n_b}{n} \delta_x \delta_y \end{aligned} \tag{4}$$

III. ORDER STATISTICS

Order statistics are one of the fundamental tools in non-parametric data analysis. They can be used to represent various statistics, such as *min*, *max*, *range*, *median*, *quantiles* and *inter-quartile mean*. Although order statistics do not suffer from numerical stability problems, computing them efficiently in MapReduce is a challenge.

Arbitrary order statistics from a set of n numbers can be computed sequentially in $O(n)$ time using the popular BFPRT algorithm [6]. There exist several efforts such as [4] that attempt to parallelize the sequential BFPRT algorithm. The core idea is to determine the required order statistic *iteratively* by *dynamically redistributing* the data in each iteration among different cluster nodes to achieve load balancing. These iterative algorithms are suited for MPI-style parallelization but they are not readily applicable to MapReduce, as they require multiple MapReduce jobs with multiple disk reads and writes. Furthermore, message passing in MapReduce can only be achieved through the heavy-weight shuffling mechanism. In SystemML, we therefore devised a sort-based algorithm by leveraging Hadoop's inherent capability to sort large set of numbers. This algorithm needs only one full MapReduce job to sort the input data, plus one partial scan of the sorted data to compute the required order statistics. Note that there have also been studies on parallel approximate order statistics algorithms [8], but in this paper, we focus only on algorithms for exact order statistics.

Sort-Based Order Statistics Algorithm: This algorithm consists of three phases. The first two phases are inspired by Yahoo's TeraSort algorithm [1].

Sample Phase: This phase samples N_s items from the input data, which are then sorted and divided evenly into r partitions,

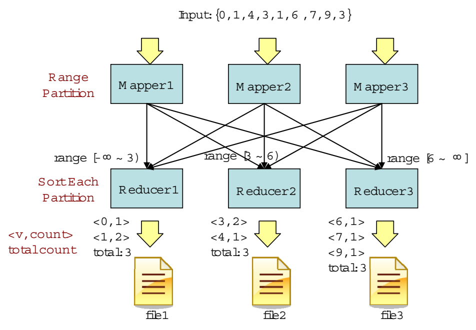

Fig. 1. Sort-Based Order Statistics Algorithm

where r is the number of reducers. The boundary points are used for range partitioning in the next phase.

Sort Phase: As shown in Figure 1, this phase is a MapReduce job that reads the input data, and uses the results from the previous phase to range partition the data. Each range is assigned to a different reducer, which sorts the unique values and keeps the number of occurrences for each unique value. Each reducer also computes the total number of data items in its range.

Selection Phase: For a given set of required order statistics, the output of sort phase (r sorted HDFS files and number of items in each file) is used to identify the appropriate file(s) that need to be scanned. If multiple order statistics reside in a single file, the scan cost can be shared. Furthermore, different files are scanned concurrently for improved efficiency.

IV. EXPERIMENTS

A. Experimental Setup

Experiment Cluster: The experiments were conducted with Hadoop 0.20 [2] on a cluster with 5 machines as worker nodes. Each machine has 8 cores with hyperthreading enabled, 32 GB RAM and 2 TB storage. We set each machine to run 15 concurrent mappers and 10 concurrent reducers.

Experiment Data Sets: There exist several benchmark data sets to assess the accuracy of numerical algorithms and software, such as NIST StRD [3]. However, these benchmarks mostly provide very small date sets. For example, the largest data set in NIST StRD contains only 5000 data points. To test the numerical stability of distributed algorithms, we generated large synthetic data sets similar to those in NIST StRD. Our data generator takes the data size and the value range as inputs, and generates values from uniform distribution. For our experiments, we created data sets with different sizes (10million to 1billion) whose values are in the following 3 ranges, R1:[1.0 – 1.5), R2:[1000.0 – 1000.5) and R3:[1000000.0 – 1000000.5).

Accuracy Measurement: In order to assess the numerical accuracy of the results produced by any algorithm, we need the true values of statistics. For this purpose, we rely on Java $BigDecimal$ that can represent arbitrary-precision signed decimal numbers. We implemented the naive algorithms for all statistics using Java $BigDecimal$ with precision 1000. With such a high precision, results of all mathematically equivalent algorithms should approach closely to the true value. We implemented naive recursive summation for sum, sum divided by count for mean, one-pass algorithms for higher-order statistics as shown in Table II, and textbook one-pass algorithm for covariance. We consider obtained results as the "true values" of these statistics.

We measure the accuracy achieved by different algorithms using the Log Relative Error (LRE) metric described in [14]. If q is the computed value from an algorithm and t is the true value, then LRE is defined as

$$LRE = -\log_{10} |\frac{q-t}{t}|$$

LRE measures the number of significant digits that match between the computed value from the algorithm q and the true value t. Therefore, a higher value of LRE indicates that the algorithm is numerically more stable.

TABLE II
TEXTBOOK ONE-PASS ALGORITHMS FOR HIGHER-ORDER STATISTICS

	Equations for 1-Pass Algorithm
variance	$\frac{1}{n-1}S_2 - \frac{1}{n(n-1)}S_1^2$
std	$(variance)^{\frac{1}{2}}$
skewness	$\frac{S_3 - \frac{3}{n}S_1S_2 + \frac{2}{n^2}S_1^3}{n \times std \times variance}$
kurtosis	$\frac{S_4 - \frac{4}{n}S_3S_1 + \frac{6}{n^2}S_2S_1^2 - \frac{3}{n^3}S_1^4}{n \times (variance)^2} - 3$

$S_p = \sum_{i=1}^{n} x_i^p$, which can be easily computed in one pass.

B. Numerical Stability of Univariate Statistics

In this section, we demonstrate the numeric stability of SystemML in computing a subset of univariate statistics.

Table III lists the accuracy (LRE values) of results produced by different algorithms for sum and $mean$. For summation, we compare the MapReduce Kahan summation used in SystemML against the naive recursive summation and the sorted summation. The latter two algorithms are adapted to the MapReduce environment. In case of naive recursive summation, mappers compute the partial sums using recursive summation, which are then aggregated in the reducer. In case of sorted summation, we first sort the entire data on MapReduce using the algorithm described in Section III, and then apply the adapted naive recursive summation on the sorted data. As shown in Table III, SystemML consistently produces more accurate results than the other two methods. The accuracies from naive recursive summation and the sorted summation are comparable. In terms of runtime performance, our MapReduce Kahan summation and the naive recursive summation are similar, but the sorted summation is up to 5 times slower as it performs an explicit sort on the entire data. Similarly, the accuracies obtained by SystemML for mean are consistently better than naive "sum divided by count" method.

The accuracy comparison for higher-order statistics is shown in Table IV. In SystemML, we employ the algorithms presented in Section II-C to compute required central moments, which are then used to compute higher-order statistics. We compare SystemML against the naive textbook one-pass methods (see Table II). As shown in Table IV, SystemML attains more accurate results for all statistics. The difference between the two methods in case of higher-order statistics is much more pronounced than that observed for sum and mean from Table III. This is because the round-off and truncation errors get magnified as the order increases. It is important to note that for some data sets in ranges R2 and R3, the higher-order statistics computed by the naive method are grossly erroneous (0 digits matched). More importantly, in some cases, the naive method produced negative values for variance, which led to undefined values for standard deviation, skewness and kurtosis (shown as NA in Table IV).

The value range has a considerable impact on the accuracy of univariate statistics. Even though R1, R2, and R3 have the same delta (i.e., the difference between minimum and maximum value), the accuracies obtained by all the algorithms drop as the magnitude of values increases. A popular technique to address this problem is to shift all the values by a constant, compute the statistics, and add the shifting effect back to the result. The chosen constant is typically the minimum value or the mean (computed or approximate). Chan *et al.* showed that such a technique helps in computing statistics with higher accuracy [7].

C. Numerical Stability of Bivariate Statistics

We now discuss the numerical accuracy achieved by SystemML for bivariate statistics. We consider two types of statistics: *scale-categorical* and *scale-scale*. In the former type, we compute *Eta*[1] and *ANOVA-F*[2] measures, whereas in the latter case, we compute *covariance* and *Pearson correlation (R)*[3]. For scale variables, we use data sets in value ranges R1, R2 and R3 that were described in Section IV-A. For categorical variables, we generated data in which 50 different categories are uniformly distributed.

For computing these statistics, SystemML relies on numerically stable methods for *sum*, *mean*, *variance* and *covariance* from Section II, whereas the naive method in comparison uses the naive recursive summation for sum, sum divided by count for mean, and textbook one-pass algorithms for variance and covariance.

The LRE values obtained for scale-categorical statistics are shown in Table V. From the table, it is evident that the statistics computed in SystemML have higher accuracy than the ones from the naive method. It can also be observed that the accuracy achieved by both methods reduces as the

[1]Eta is defined as $(1 - \frac{\sum_{r=1}^{R}(n_r-1)\sigma_r^2}{(n-1)\sigma^2})^{\frac{1}{2}}$, where R is the number of categories, n_r is the number of data entries per category, σ_r^2 is the variance per category, n is the total number of data entries, and σ^2 is the total variance.

[2]ANOVA-F is defined as $\frac{\sum_{r=1}^{R} n_r(\mu_r-\mu)^2}{\sum_{r=1}^{R}(n_r-1)\sigma_r^2} . \frac{n-R}{R-1}$, where R is the number of categories, n_r is the number of data entries per category, μ_r is the mean per category, σ_r^2 is the variance per category, n is the total number of data entries, and μ is the total mean.

[3]Pearson-R is defined as $\frac{\sigma_{xy}}{\sigma_x\sigma_y}$, where σ_{xy} is the covariance, σ_x and σ_y are standard deviations.

TABLE III
NUMERICAL ACCURACY OF SUM AND MEAN (LRE VALUES)

	Size (million)	Sum			Mean	
Range		SystemML	Naive	Sorted	SystemML	Naive
R1	10	16.1	13.5	16.1	16.7	13.5
	100	16.3	13.8	13.6	16.2	13.8
	1000	16.8	13.6	13.5	16.5	13.6
R2	10	16.8	14.4	13.9	16.5	14.4
	100	16.1	13.4	13.4	16.9	13.4
	1000	16.6	13.1	13.9	16.4	13.1
R3	10	15.9	14.0	13.9	16.3	14.0
	100	16.0	13.1	13.4	16.9	13.1
	1000	16.3	12.9	12.2	16.5	12.9

TABLE IV
NUMERICAL ACCURACY OF HIGHER-ORDER STATISTICS (LRE VALUES)

	Size (million)	Variance		Std		Skewness		Kurtosis	
Range		SystemML	Naive	SystemML	Naive	SystemML	Naive	SystemML	Naive
R1	10	16.0	11.3	15.9	11.6	16.4	7.5	15.3	9.8
	100	16.2	11.5	16.8	11.8	14.9	7.1	15.6	9.3
	1000	16.0	11.3	16.4	11.6	14.5	6.5	15.6	8.9
R2	10	15.4	5.9	15.9	6.2	12.5	0	14.9	0
	100	15.6	5.3	15.8	5.6	12.0	0	14.9	0
	1000	16.2	4.9	16.4	5.2	12.1	0	15.2	0
R3	10	14.4	0	14.7	0	9.1	0	12.6	0
	100	12.9	0	13.2	NA	9.0	NA	13.2	NA
	1000	13.2	0	13.5	NA	9.4	NA	12.9	NA

NA represents undefined standard deviation, skewness or kurtosis due to a negative value for variance.

TABLE V
NUMERICAL ACCURACY OF BIVARIATE SCALE-CATEGORICAL STATISTICS: ETA AND ANOVA-F (LRE VALUES)

	Size (million)	Eta		ANOVA-F	
Range		SystemML	Naive	SystemML	Naive
R1	10	16.2	13.7	16.2	10.0
	100	16.6	13.7	15.6	10.0
	1000	16.5	13.6	15.8	9.9
R2	10	16.2	7.2	13.3	3.5
	100	16.6	7.4	13.4	3.7
	1000	16.5	7.9	13.4	4.3
R3	10	16.2	0	10.2	0
	100	15.9	1.9	10.0	0
	1000	16.5	1.2	10.0	0

TABLE VI
NUMERICAL ACCURACY OF BIVARIATE SCALE-SCALE STATISTICS: COVARIANCE AND PEARSON-R (LRE VALUES)

	Size (million)	Covariance		Pearson-R	
Range		SystemML	Naive	SystemML	Naive
R1 vs. R2	10	15.0	8.4	15.1	6.2
	100	15.6	8.5	15.4	6.4
	1000	16.0	8.7	15.7	6.2
R2 vs. R3	10	13.5	3.0	13.5	3.0
	100	12.8	2.8	12.7	NA
	1000	13.6	3.9	13.8	NA

NA represents undefined Pearson-R due to a negative value for variance.

magnitude of input values increases – e.g., LRE numbers for R3 are smaller than those of R1. As we move from R1 to R3, the accuracy of the naive method drops more steeply compared to SystemML. This is because the inaccuracies of total and per-category $mean$ and $variance$ quickly propagate and magnify the errors in Eta and ANOVA-F. Similar trends can be observed in case of covariance and Pearson correlation, as shown in Table VI. For the cases of R2 vs. R3 with 100 million and 1 billion data sets, the naive algorithm produces negative values for variance (see Table IV), which resulted in undefined values for Pearson-R (shown as NA in Table VI).

D. *The Impact of* KAHANINCREMENT

In this section, we evaluate the effect of using KAHANINCREMENT in the update rules of central moments (Equation 3) and covariance (Equation 4) on the accuracy of the results.

Table VII and Table VIII show the numerical accuracy achieved by the update rules using KAHANINCREMENT and basic addition for higher-order statistics and scale-scale bivariate statistics. Evidently, update rules using KAHANINCREMENT are able to produce more accurate results for all statistics across the board. In SystemML, the correction terms maintained in Kahan technique helps in reducing the effect of truncation errors.

E. *Performance of Order Statistics*

In this section, we evaluate the scalability of the sort-based order statistics algorithm presented in Section III. Script 1

TABLE VII
THE EFFECT OF KAHANINCREMENT ON THE ACCURACY OF HIGHER-ORDER STATISTICS (LRE VALUES)

	Size (million)	Variance		Std		Skewness		Kurtosis	
Range		Kahan	Basic	Kahan	Basic	Kahan	Basic	Kahan	Basic
R1	10	16.0	13.5	15.9	13.8	16.4	13.0	15.3	13.7
	100	16.2	13.7	16.8	14.0	14.9	12.5	15.6	12.8
	1000	16.0	14.1	16.4	14.4	14.5	12.1	15.6	11.8
R2	10	15.4	12.8	15.9	13.1	12.5	11.8	14.9	13.4
	100	15.6	12.5	15.8	12.8	12.0	9.7	14.9	14.3
	1000	16.2	13.8	16.4	14.1	12.1	9.3	15.2	11.8
R3	10	14.4	9.3	14.7	9.6	9.1	7.1	12.6	9.5
	100	12.9	9.5	13.2	9.8	9.0	6.8	13.2	9.7
	1000	13.2	10.3	13.5	10.6	9.4	6.3	12.9	10.0

TABLE VIII
THE EFFECT OF KAHANINCREMENT ON THE ACCURACY OF COVARIANCE AND PEARSON-R (LRE VALUES)

	Size (million)	Covariance		Pearson-R	
Range		Kahan	Basic	Kahan	Basic
R1 vs. R2	10	15.0	14.2	15.1	13.0
	100	15.6	13.3	15.4	13.0
	1000	16.0	14.6	15.7	14.2
R2 vs. R3	10	13.5	10.0	13.5	9.8
	100	12.8	10.0	12.7	10.5
	1000	13.6	11.4	13.8	10.5

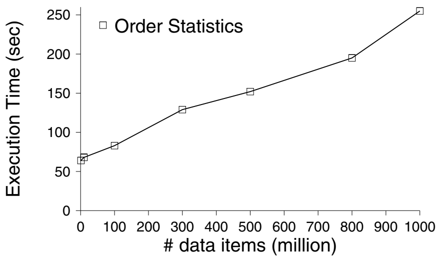

Fig. 2. Execution Time for Script 1

shows how order statistics are expressed in DML language – more details on the DML syntax can be found in [10]. The script computes the median as well as other quantiles as specified by the vector P, from the input data V. In this experiment, we fix $P = \{0.1, 0.2, 0.3, 0.4, 0.5, 0.6, 0.7, 0.8, 0.9\}$, and vary the size of V (the value range of data in V is R1). Figure 2 shows the execution time of this script as the input data size increases. For the given DML script, SystemML is able to identify that multiple different order statistics are computed on the same data set, and it accordingly performs a single sort and then computes the required order statistics. Furthermore, all the specified order statistics are selected simultaneously, in parallel.

Script 1: A Simple Script of Order Statistics
```
# input vector (column matrix)
V = read("in/V");
# a vector specifying the desired quantiles
P = read("in/P");
# compute median
median = quantile(V, 0.5);
print("median: ", median);
# compute quantiles
Q = quantile(V, P);
write(Q, "out/Q");
```

V. DISCUSSION

We now summarize the lessons learned while implementing scalable and numerically stable descriptive statistics in SystemML.

• **Many existing sequential techniques for numerical stability can be adapted to the distributed environment.**

We successfully adapted the existing sequential stable algorithms for summation, mean, central moments and covariance to the MapReduce environment. Such adaptations are empirically shown to exhibit better numeric stability when compared to commonly used naive algorithms.

• **Performance need not be sacrificed for accuracy.**

While software packages like $BigDecimal$ can be used to improve the numerical accuracy of computations, they incur significant performance overhead – we observed up to 5 orders of magnitude slowdown depending on the exact operation and precision used. Similarly, the *sorted sum* technique that is widely used in sequential environments is not able to achieve similar accuracy when adapted to a distributed environment. Furthermore, its performance is hindered by the fact that the entire data has be sorted up front. In contrast, our stable algorithms for summation, mean, covariance, and higher order statistics achieve good accuracy without sacrificing the runtime performance – they make a single scan over the input data, and achieve comparable runtime performance with the unstable one-pass algorithms.

• **Shifting can be used for improved accuracy.**

When all the values in the input data set are of large magnitude, it is useful to shift the elements by a constant (minimum value or approximate mean) prior to computing any statistics. This preprocessing technique helps in reducing the truncation errors, and often achieves better numerical accuracy. In the absence of such preprocessing, as shown in Sections IV-B & IV-C, the accuracy of statistics degrades as the magnitude of input values increases (e.g., as the value range changes from R1 to R3).

• **Divide-and-conquer design helps in scaling to larger data sets while achieving good numerical accuracy.**

All the stable algorithms discussed in this paper operate in a divide-and-conquer paradigm, in which the partial results are computed in the mappers and combined later in the reducer. These algorithms partitions the work into smaller pieces, and hence they can scale to larger data sets while keeping the relative error bound independent of the input data size. For example, the sequential version of Kahan summation algorithm guarantees that the relative error bound is independent of the input data size as long as the *total number* of elements is in the order of 10^{16}. In contrast, the MapReduce version of Kahan summation algorithm can provide similar guarantees as long as the data size processed by *each* mapper is in the order of 10^{16}. In the words, the parallel version of the algorithm can scale to larger data sets without having a significant impact on the error bound. Here, we assume that the number of mappers is bounded by a constant which is significantly smaller than the input data size. While there is no formal proof of such a result for covariance and other higher-order statistics, we expect the distributed algorithms for these statistics to scale better than their sequential counterparts.

• **Kahan technique is useful beyond a simple summation.**

The strategy of keeping the correction term, as in Kahan summation algorithm, helps in alleviating the effect of truncation errors. Beyond the simple summation, we found this technique to be useful in computing stable values for other univariate and bivariate statistics, including mean, variance, covariance, Eta, ANOVA-F etc.

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Appendix A
Proof of Error Bound for MapReduce Kahan Summation Algorithm

The relative error bound for the MapReduce Kahan summation algorithm is $\frac{|E_n|}{|S_n|} \leq [4u + 4u^2 + O(mu^2) + O(\frac{n}{m}u^2) + O(mu^3) + O(\frac{n}{m}u^3) + O(nu^4)]\kappa_X$.

Proof: As each of the m mappers uses Kahan algorithm, the k-th mapper has the error bound $E_{n_k} = |\hat{S}_{n_k} - S_{n_k}| \leq (2u + O(n_k u^2)) \sum_{i=1}^{n_k} |x_{k,i}|$, where n_k is the number of data items process by this mapper. As n_k is in $O(\frac{n}{m})$, we can simply derive $E_{n_k} \leq (2u + O(\frac{n}{m}u^2)) \sum_{i=1}^{n_k} |x_{k,i}|$.

Each mapper generates $\hat{S}_{n_k}$ with its correction term. In the single reducer, we again run the Kahan sum algorithm on these m data items, therefore, we get derive the error incurred in the reducer as follows:

$$
\begin{aligned}
&|\hat{S}_n - \sum_{i=1}^{m} \hat{S}_{n_k}| \\
\leq &(2u + O(mu^2)) \sum_{k=1}^{m} |\hat{S}_{n_k}| \\
\leq &(2u + O(mu^2)) \sum_{k=1}^{m} (|S_{n_k}| + E_{n_k}) \\
\leq &(2u + O(mu^2)) \sum_{k=1}^{m} (\sum_{i=1}^{n_k} |x_{k,i}| + (2u + O(\frac{n}{m}u^2)) \sum_{i=1}^{n_k} |x_{k,i}|) \\
\leq &(2u + O(mu^2))(1 + 2u + O(\frac{n}{m}u^2)) \sum_{i=1}^{n} |x_i| \\
\leq &(2u + 4u^2 + O(mu^2) + O(mu^3) + O(\frac{n}{m}u^3) + O(nu^4)) \sum_{i=1}^{n} |x_i|
\end{aligned}
$$

We can now derive the upper bound on the relative error for MapReduce Kahan summation as follows:

$$
\begin{aligned}
&|\hat{S}_n - S_n| = |\hat{S}_n - \sum_{i=1}^{m} S_{n_k}| \\
=&|\hat{S}_n - \sum_{i=1}^{m} \hat{S}_{n_k} + \sum_{i=1}^{m} \hat{S}_{n_k} - \sum_{i=1}^{m} S_{n_k}| \\
\leq&|\hat{S}_n - \sum_{i=1}^{m} \hat{S}_{n_k}| + |\sum_{i=1}^{m} \hat{S}_{n_k} - \sum_{i=1}^{m} S_{n_k}| \\
\leq&|\hat{S}_n - \sum_{i=1}^{m} \hat{S}_{n_k}| + \sum_{i=1}^{m} |\hat{S}_{n_k} - S_{n_k}| \\
\leq&|\hat{S}_n - \sum_{i=1}^{m} \hat{S}_{n_k}| + \sum_{i=1}^{m} ((2u + O(\frac{n}{m}u^2)) \sum_{i=1}^{n_k} |x_{k,i}|) \\
\leq&(2u + 4u^2 + O(mu^2) + O(mu^3) + O(\frac{n}{m}u^3) + O(nu^4)) \sum_{i=1}^{n} |x_i| \\
&+ (2u + O(\frac{n}{m}u^2)) \sum_{i=1}^{n} |x_i| \\
\leq&(4u + 4u^2 + O(mu^2) + O(\frac{n}{m}u^2) + O(mu^3) + O(\frac{n}{m}u^3) + O(nu^4)) \sum_{i=1}^{n} |x_i|
\end{aligned}
$$

As a result, the relative error bound for MapReduce Kahan summation is $\frac{|E_n|}{|S_n|} \leq [4u + 4u^2 + O(mu^2) + O(\frac{n}{m}u^2) + O(mu^3) + O(\frac{n}{m}u^3) + O(nu^4)]\kappa_X$. ■