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Report Title

Final Report: Data-Based Detection of Potential Terrorist Attacks: Statistical and Graphical Methods

ABSTRACT

This report describes results of research contained in published papers and technical reports on statistical methods in the identification of rare events such as those that arise in terrorist attacks. Because data for national security operations are highly classified, techniques are developed on massive data containing rare events that arise in particle physics, internet communications, and genomics. Results include: (a) useful graphical displays; (b) conditioning high-dimensional data; (c) penalized regression estimators to filter out irrelevant variables.

List of papers submitted or published that acknowledge ARO support during this reporting period. List the papers, including journal references, in the following categories:

(a) Papers published in peer-reviewed journals (N/A for none)

Beall, Jeffrey; Kafadar, Karen:
"The Proportion of NUC Pre-56 Titles Represented in OCLC
WorldCat," *College & Research Libraries* 66(5), 431-435 (2005).

Kafadar, Karen; Wegman, Edward J.:
"Visualizing 'typical' and 'exotic' Internet traffic data."
Computational Statistics and Data Analysis 50, 3721-3743 (2006).

Spiegelman, Clifford H.; Kafadar, Karen:
"Data Integrity and the Scientific Method: The Case of Bullet
Lead Data as Forensic Evidence (with discussion),"
Chance 19(2), 17-25 (2006).

Saha, Nilanjan; Watson, Layne T.; Kafadar, Karen; Onufriev, Alexey;
Ramakrishnan, Naren; Vasquez-Robinet, Cecilia; Watkinson, Jonathan:
"A General Probabilistic Model of the PCR Process,"
Applied Mathematics and Computation 182(1), 232--243 (2006).

Du, Yunzhi; Davisson, Muriel T.; Kafadar, Karen; Gardiner, Katheleen:
"A-to-I pre-mRNA editing of the serotonin 2C receptor: Comparisons
among inbred mouse strains,"
Gene 382: 39--46 (1 Nov 2006);
available online at <http://www.sciencedirect.com>.

Beall, Jeffrey; Kafadar, Karen:
"Measuring Typographical Errors' Impact on Retrieval in
Bibliographic Databases (invited),"
Cataloging & Classification Quarterly 44(3/4), 197-211 (2007).

Saha, Nilanjan; Watson, Layne T.; Kafadar, Karen; Ramakrishnan, Naren;
Onufriev, Alexey; Rao Mane, Shrinivas; Vasquez-Robinet, Cecilia:
"Validation and Estimation of Parameters for a General Probabilistic
Model of the PCR Process,"
Journal of Computational Biology 14(1): 97-112 (2007).

Bjork, Kathe E.; Kafadar, Karen:
"Systematic order dependent effect in expression values, variance,
detection calls and differential expression in Affymetrix GeneChips(R),"
Bioinformatics 2007; doi: 10.1093/bioinformatics/btm450

Beall, Jeffrey; Kafadar, Karen:
"Measuring the Extent of the Synonym Problem in Full-text Searching,"
Evidence Based Library and Information Practice 2008 3(4), 18-33.

Gehrke, Allison; Sun, Shaojun; Kurgan, Lukasz A.; Ahn, Natalie G.;
"Improved machine learning methods for analysis of gas phase
chemistry of peptides,"
Bioinformatics 2008 9:515; doi:10.1186/1471-2105-9-515.

Kafadar, K.; Bjork, K.E.:
"Microarray analysis",
In: *Encyclopedia of Quantitative Risk Assessment*, Volume 1
(Edward L. Melnick and Brian S. Everitt, eds.), Wiley, 2008.

Gonzales, Ralph; Corbett, Kitty K.; Wong, Shale; Glazner, Judith;

Gershman, Kenneth; Deas, Ann; Leeman-Castillo, Bonnie A.; Maselli, Judith H.; Severt-Kuhlmann, Ann; Wigton, Robert S.; Flores, Estevan; Kafadar, Karen:
"Get Smart Colorado": Impact of a Mass Media Campaign to Improve Antibiotic Use,"
Medical Care 46(6), 597-605 (2008).

Kafadar, K.; Prorok, P.C.:
"Effect of length-biased sampled sojourn times on the survival distribution in randomized cancer screening trials,"
Statistics in Medicine, 28:2116-2146, 2009.

Number of Papers published in peer-reviewed journals: 12.00

(b) Papers published in non-peer-reviewed journals or in conference proceedings (N/A for none)

Number of Papers published in non peer-reviewed journals: 0.00

(c) Presentations

(All presentations at meetings and seminars are shown)

Invited seminar,
Statistical Tests for Bullet Lead Comparisons,
Department of Statistics,
North Carolina State University, 21 March 2006.

Topics contributed paper,
Letter value plots,
Interface Symposium, Pasadena, May 2006;
Joint Statistics Meetings, Seattle, August 2006.

Seminar,
Length biased sampling in randomized screening trials,
Statistics Colloquium, CU-Denver, September 2006.

Seminar,
Measuring the effect of Length biased sampling,
Mathematical Sciences Section, National Security Agency,
19 September 2006.

Contributed paper,
Letter value plots,
Army Conference on Applied Statistics, Raleigh, October 2006.

Invited seminar,
Statistical Tests for Bullet Lead Comparisons,
Department of Statistics,
Florida State University, 7 December 2006.

Seminar,
Length biased sampling in randomized screening trials,
Department of Statistics, Texas A&M University, 22 January 2007.

Invited Member Presentation,
Statistical issues for NRC's Bullet Lead Committee,
Committee on National Statistics, 9 February 2007.

Invited seminar,
Statistical Tests for Bullet Lead Comparisons,
Department of Mathematics, Butler University, 7 March 2007.

Bernard Flury Lecture,
Statistical Tests for Bullet Lead Comparisons,
Department of Statistics,
Indiana University, 8 March 2007.

Plenary lecture,
Statistics in Forensic Sciences (with C.S. Spiegelman),
Army Conference on Applied Statistics, October 2007.

Neyman seminar,
Statistical Tests for Bullet Lead Comparisons,
UC-Berkeley, October 2007.

Invited seminar,

Statistical Tests for Bullet Lead Comparisons,
ASA San Francisco Bay Chapter, Jan 2008.

Invited seminar,
Statistical Tests for Bullet Lead Comparisons,
Washington Statistical Society, Feb 2008.

Invited seminar,
Massive Data Sets in High-Energy Physics,
Univ of California-San Francisco, Apr 2008.

Invited speaker,
Massive Data Sets in Scientific Applications,
Statistics Conference, West Point Academy, 17 Apr 2008.

Contributed paper,
Statistical Considerations in Large-Scale Screening
Programs: Impacts on the Public,
Joint Statistics Meetings, Denver, Aug 2008.

Contributed paper,
Massive Data Sets in High-Energy Physics.
Joint Statistics Meetings, Denver, Aug 2008.

Plenary lecture,
Statistical methods for massive data in physics and genomics,
International Conference on Robust Statistics,
Antalya, Turkey, September 2008.

Contributed paper,
Massive Data Sets in High-Energy Physics,
Army Conference on Applied Statistics, Lexington, VA, 23 Oct 2008.

Invited seminar,
Statistics in the Forensic Sciences,
Dept of Statistics, Univ of Illinois Urbana-Champaign, 22 Jan 2009.

Invited seminar,
Statistical methodology for massive data sets,
Department of Statistics, Stern School of Business,
New York University, 27 Feb 2009.

Invited seminar,
Statistical methodology for randomized cancer screening trials,
Department of Statistics and Actuarial Sciences,
University of Iowa, 9 Apr 2009.

Invited (with A. Mazza),
Statistical issues in the evaluation of fingerprint evidence,
Annual meeting of the Scientific Working Group on Friction
Ridge Analysis, Study and Technology, St. Paul MN, May 2009.

Invited,
Statistical methodology for high-energy physics data,

Jet Propulsion Laboratory, 19 May 2009.

Invited seminar,
Challenges in the statistical analysis of massive data sets,
Computer Science, Indiana University, 7 Oct 2009.

Invited seminar,
Length biased sampling in randomized screening trials,
Department of Statistics, Purdue University, 8 Oct 2009.

Contributed paper (with A.M. Santos, presenter):
Robust estimation of mixtures of long-tailed distributions.
Army Conference on Applied Statistics, Phoenix, 22 Oct 2009.

Contributed paper,
Statistical issues in the comparison of multi-dimensional profiles,
Army Conference on Applied Statistics, Phoenix, 23 Oct 2009.

Invited seminar,
Statistical issues in the analysis of massive data sets,
Dept of Statistics, Kansas State University, 11 Mar 2010.

Invited seminar,
Statistical analysis of randomized cancer screening trials,
ASA Chapter, Kansas, 11 Mar 2010.

Invited presentation,
"The NAS Report on Forensic Science,"
Los Angeles County Public Defender's Workshop on Forensic Training,
Los Angeles, 20 Mar 2010.

Invited presentation,
The NAS Report on Forensic Science,
Chesapeake Bay Regional Meeting of the International
Association for Identification, Norfolk VA, 25 Mar 2010.

Invited presentation,
Statistical considerations in evaluating forensic science methods,
National Association of Criminal Defense Lawyers, Atlanta, 15 Apr 2010.

Invited presentation,
Statistical considerations in evaluating forensic science methods,
District Court Federal Judges Workshop, 6 May 2010.

Invited presentation,
Effect of influential observations on penalized regression estimators,
International Conference on Robust Statistics, Prague, 29 Jun 2010.

Invited presentation,
Statistical issues in comparing multidimensional profiles,
International Symposium on Business and Industrial Statistics,
Portoroz Slovenia, 8 Jul 2010.

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Non Peer-Reviewed Conference Proceeding publications (other than abstracts):

Peer-Reviewed Conference Proceeding publications (other than abstracts):

Peskin, Adele P.; Kafadar, K.; Santos, A.M.; Haemer, Gillian G.:
"Robust Volume Calculations of Tumors of Various Sizes,"
Proceedings of the 2009 International Conference on
Image Processing, Computer Vision, and Pattern Recognition.
(Refereed; CD).

Peskin, A.P.; Kafadar, K.; Dima, A.; Bernal, Javier; Gilsinn, D.:
"Synthetic Lung Tumor Data Sets for Comparison of Volumetric Algorithms,"
Proceedings of the 2009 International Conference on
Image Processing, Computer Vision, and Pattern Recognition.
(Refereed; CD).

(d) Manuscripts

Hofmann, Heike; Kafadar, Karen; Wickham, Hadley:
Letter value plots.

Kafadar, K.; Jacobsen, R.G.:
Statistical issues in the analysis of massive data in
high-energy physics experiments.

Heltshe, Sonya; Kafadar, Karen; Prorok, Philip C.:
Quantification of Length Biased Sampling in Randomized Screening Trials.

Patents Submitted

Patents Awarded

Graduate Students

NAME	PERCENT SUPPORTED
Kathe E. Bjork	0.10
Sonya Heltshe	0.15
A. Melissa Santos	0.25
Mark Werner	0.50
Armen Zakharyan	0.00
Gregory Lobser	0.00
FTE Equivalent:	1.00
Total Number:	6

Names of Post Doctorates

NAME	PERCENT SUPPORTED
FTE Equivalent:	
Total Number:	

Names of Faculty Supported

<u>NAME</u>	<u>PERCENT SUPPORTED</u>	National Academy Member
Karen Kafadar	0.10	No
FTE Equivalent:	0.10	
Total Number:	1	

Names of Under Graduate students supported

<u>NAME</u>	<u>PERCENT SUPPORTED</u>
FTE Equivalent:	
Total Number:	

Student Metrics

This section only applies to graduating undergraduates supported by this agreement in this reporting period

The number of undergraduates funded by this agreement who graduated during this period:	0.00
The number of undergraduates funded by this agreement who graduated during this period with a degree in science, mathematics, engineering, or technology fields:.....	0.00
The number of undergraduates funded by your agreement who graduated during this period and will continue to pursue a graduate or Ph.D. degree in science, mathematics, engineering, or technology fields:.....	0.00
Number of graduating undergraduates who achieved a 3.5 GPA to 4.0 (4.0 max scale):.....	0.00
Number of graduating undergraduates funded by a DoD funded Center of Excellence grant for Education, Research and Engineering:.....	0.00
The number of undergraduates funded by your agreement who graduated during this period and intend to work for the Department of Defense	0.00
The number of undergraduates funded by your agreement who graduated during this period and will receive scholarships or fellowships for further studies in science, mathematics, engineering or technology fields:	0.00

Names of Personnel receiving masters degrees

<u>NAME</u>	
Stephen Fisher	
Jason Gonzales	
A. Melissa Santos	
Total Number:	3

Names of personnel receiving PhDs

<u>NAME</u>	
Kathe E. Bjork	
Sonya Heltshe	
Gregory Lobser	
Armen Zakharyan	
Total Number:	4

Names of other research staff

<u>NAME</u>	<u>PERCENT SUPPORTED</u>	
Dana Franklin	0.50	No
FTE Equivalent:	0.50	
Total Number:	1	

Inventions (DD882)

Final Report: Data-Based Detection of Potential Terrorist Attacks:

Statistical and Graphical Methods

June 2010

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Executive Summary

This research has developed methods for analysis and display of massive data. A series of issues were studied: graphical methods (letter value plots), dimension reduction, evaluation of forensic science methods, analysis of gene expression data, and effects of length biased sampling. This report summarizes the findings on each of these topics.

1 Statement of problem studied: Methods to identify outliers in massive data streams

Statistical algorithms have been developed to detect unusual events or aberrations that may indicate serious problems. The contexts for which these algorithms have been developed generally involve very large numbers of records but often only a few outcome variables and covariates: for example, high incidence of infectious diseases (possible epidemics), excessive charges on a credit card or telephone (possible stolen card), or high levels of environmental pollutants. Another simplifying feature of the data for these contexts is the ability to stratify the data into reasonably homogeneous groups; e.g., by disease or disease category; by individual or family; by geographical locale. The challenges today with massive data arise because of the disparate nature, source, and type of data, such as passengers with accompanying baggage that have checked in for a flight, syndromic surveillance, or computer operations or Internet sessions. The research that was conducted during the period of this grant solves problems and develops methodology needed for the analysis of these types of data.

The specific tasks documented in the proposal, and the results of the tasks, are outlined below.

1. *Continue collaborations with Professor Wegman at George Mason University on the development of “evolutionary graphical displays” through summer visits and using GMU’s Internet traffic data.*

The result of this collaboration was the published article:

Kafadar, Karen; Wegman, Edward J.: ”Visualizing ‘typical’ and ‘exotic’ Internet traffic data.”
Computational Statistics and Data Analysis 50, 3721-3743 (2006).

In this article, we propose new displays that can be used readily by non-technical personnel for monitoring Internet communications. We develop skyline plots, moving histograms, and use waterfall diagrams (Marchette and Wegman 2004).

2. *Initiate research on the development of methods of analysis (metrics, information, residuals) on graphical objects.*

Research on this topic evolved to address methods for analyzing segmentation methods of tumor image data, needed for accurate and precise estimates of tumor volumes. The work involved collaborations with Dr. A.P. Peskin and colleagues at the National Institute of Standards and Technology. Two refereed conference proceedings were published:

- Peskin, Adele P.; Kafadar, K.; Santos, A.M.; Haemer, Gillian G.: “Robust Volume Calculations of Tumors of Various Sizes,” Proceedings of the 2009 International Conference on Image Processing, Computer Vision, and Pattern Recognition. (Refereed; CD).

Many advances in medicine today require the accurate reading of computerized tomographic (CT) images of the body. Tumors in the lung, for example, are classified according to their detected growth, i.e. change in volume, over a period of time. CT data are collected as sets of three-dimensional grid points. Tumors are often so small that a large proportion of the pixels that represent the tumors lie near the tumor surfaces. If an edge of a tumor lies between two pixel locations, radiologists must determine which of those pixels should be included in a measurement of the tumor size, determinations which can have large effects on estimated tumor volumes. Current techniques to measure these “partial volumes,” or 3-D voxels in the grid that are only partially filled, in this case by a tumor in a scan of the lung, vary widely in resulting tumor volume measurements. We present a statistical method that leads to accurate estimates of these volumes.

- Peskin, Adele P.; Kafadar, K.; Dima, Alden; Bernal, Javier; Gilsinn, David: “Synthetic Lung Tumor Data Sets for Comparison of Volumetric Algorithms,” Proceedings of the 2009 International Conference on Image Processing, Computer Vision, and Pattern Recognition. (Refereed; CD).

The change in pulmonary nodules over time is an important indicator of malignant tumors. It is therefore important to be able to measure change in the size of tumors from

computed tomography (CT) data taken at different times and on potentially different CT machines. A particular tumor may or may not be divided into slices at exactly the same places on two different sets of scans. The pixel distributions and average background values may also not be the same between two different sets of data. Standardized sets of data are needed to compare techniques for calculating tumor volumes and/or the change in tumor size between two sets of data. Combining phantom data with realistic lung data could provide realistic standardized data sets, which include many of the measurement challenges that are not available in pure phantom data alone. We present a set of synthetic lung tumor data in which synthetic tumors of known volume are embedded in real lung CT data in different background settings in the lung.

3. *Study the robustness (validity, efficiency) of Hotelling's T^2 statistic to misspecified covariance matrix as part of the research into the development of methods of analysis on graphical objects that contain multiple features.*

The problem of accurate and precise estimates of covariance matrices among large numbers of variables leads to the need for dimension reduction methods. Historically, the method of principal components has provided a reduced set of orthogonal variables that are linear combinations of the original variables. These principal components are useful but often not insightful. Alternative methods include modifying the coefficients to “meaningful” values, or penalized regression estimators as a way of shrinking (to zero) the coefficients for potentially insignificant variables. We take the latter approach in this research. This work involved collaborations with Guilherme V. Rocha, and early efforts have been presented at two recent conferences:

- Effect of influential observations on penalized regression estimators, International Conference on Robust Statistics, Prague, 29 Jun 2010.
- Invited presentation, Statistical issues in comparing multidimensional profiles, International Symposium on Business and Industrial Statistics, Portoroz Slovenia, 8 Jul 2010.

This research demonstrates that ordinary penalized regression estimators, such as ridge regression (L_2 loss function: minimize the sum of squared residuals; L_2 penalty function on

the coefficients: sum of the squared coefficients constrained to be less than a pre-selected limit), or Lasso (Tibshirani 1996: L_2 loss function; L_1 penalty function), can be influenced by outliers. A good compromise that pays less attention to outliers, but performs well with both Gaussian and long-tailed (Cauchy) data, combines the use of Lasso’s L_1 penalty function with an L_1 loss function.

4. *Work with Professor Robert L. Jacobsen (U.C. Berkeley) in the development of methods and searches for “outliers” defined by specific combinations of events in massive high-energy physics databases.*

New statistical methods arise in response to new data types encountered in various disciplines; e.g., design of experiments to identify influential factors in plant and animal studies, survival analysis and sequential analysis of data from medical investigations, detection of echoes in long-range time series data, nonparametric and robust methods for non-Gaussian data, multiple comparisons to address multiple hypothesis tests. Advances in both the scientific discipline and statistics result from successful collaborations between the scientific investigators with the data and the statisticians with the tools to develop methods for analyzing them. These opportunities exist for collaborations between statisticians and high-energy experimental particle physicists, with high potential for significant research advances in both fields. Particle physics experiments produce massive amounts of streaming data from the occurrence of “events” (collisions between particles or other types of particle activity), whose constituents are measured, recorded, and saved in huge data bases. As newer and faster accelerators lead to ever-increasing amounts of data, the increasing amounts of data demand the development of efficient statistical methods to identify subtle effects amidst immense, but largely already well-established, effects. We outline in this article the framework under which experimental physicists conduct their investigations and review areas where statistics has been applied already to advance knowledge in the field. We then focus on current challenges and provide an approach to study massive data sets with the goal of identifying a very small fraction of unusual “target” events. The analysis framework likely will be applicable to massive data problems in fields such as protein identification, financial and marketing applications, and public safety surveillance systems.

2 Cybersecurity: Monitoring Internet Traffic Data

This research was conducted with Professor Edward J. Wegman at George Mason University (GMU). Table 1 shows some of the information contained in the TCP/IP headers in a sample of ten records from the 135,605 sessions captured during the course of one hour of Internet traffic at GMU. (This hour occurred during exam week, a relatively quiet time on the campus; typical one-hour data sets during the semester contained many more than 135,605 sessions.) Column 1 labeled **time** denotes the clock time at which the Internet session began; **length** represents the length of the session in seconds; **SIP** and **DIP** are the source and destination ports, respectively; **DPort** and **SPort** are the destination and source port numbers, respectively; and **Npacket** and **Nbyte** indicate the number of packets and number of bytes transferred in the session. The five-number summary and the 10th and 90th percentiles for each column (minimum, lower 10%, lower fourth, median, upper fourth, upper 10%, maximum) are listed in Table 2. The “size” variables are all highly correlated and very highly skewed towards the upper end; the distance between the 90th percentile and the maximum is huge. All benefited from a logarithmic transformation (specifically, $\log(1 + \sqrt{x})$, so small values are not spread out as far as large values are pulled in). One session involved over 35 million bytes, and almost 66,000 packets, although sessions of 1,832 bytes and 12 packets were more typical. With over 135,000 sessions in only one relatively quiet hour and dozens of variable on each, success at monitoring potential cyberattacks will require graphical displays and methods of visually analyzing such displays, i.e., “visual analytics” (Wegman 2004).

Table 1: Sample of Internet traffic data from George Mason University

	time	length	SIP	DIP	DPort	SPort	Npacket	Nbyte
1	39603.64	0.23	4367	54985	443	1631	9	3211
2	39603.64	0.27	18146	9675	3921	25	15	49
3	39603.65	0.04	18208	28256	1255	80	6	373
4	39603.65	1389.10	24159	17171	23	1288	845	5906
5	39603.65	373.99	60315	37727	2073	80	1759	834778
6	39603.65	0.13	28256	18208	80	1256	10	816
7	39603.65	1498.11	25699	4837	9593	80	65803	35661821
8	39603.65	0.04	18208	28256	1251	80	5	373

9	39603.66	122.38	54985	4179	1298	443	99	85559
10	39603.66	0.13	28256	18208	80	1257	10	816
11	39603.66	0.00	18464	28256	1253	80	3	0
12	39603.67	33.17	22859	7765	1269	80	20	9221
13	39603.67	1270.91	17899	21649	2318	8028	29216	17438688
14	39603.67	237.70	7693	40669	1680	80	2553	637466
15	39603.68	1.01	14853	9675	3920	25	18	5415

Table 2: Summary statistics from Internet traffic data set (135,605 sessions)

	time	duration	SIP	DIP	DPort	SPort	Npacket	Nbyte
minimum	39603.64	0.00	259	259	20	20	2	0
lower 10%	39937.68	0.20	4930	4024	80	1187	9	568
lower 4th	40507.09	0.32	9765	8705	80	1369	10	860
median	41435.55	0.58	20258	25164	80	1849	12	1832
upper 4th	42326.46	3.77	41282	45900	80	3681	21	7697
upper 10%	42857.49	21.45	62754	58202	80	10000	45	25161
maximum	43201.26	3482.50	65276	65262	10000	10000	65803	35661821
#(unique values)	104268	9101	3548	5427	380	6742	1056	29876

The first task in multivariate outlier detection is to identify in any given set of circumstances what might be considered “unusual.” For example, in the one-hour data set from George Mason University, 85.6% of the records were destined for the web (destination port 80 reserved for `http`); another 8.6% were targeted for secure web encryption (destination port 443 reserved for `https`). The analysis in Kafadar and Wegman (2006) uncovered patterns in the data that indicated the need to combine *sessions* into *activities* (collections of sessions all related to a single activity). This combination needs to be done robustly due to the potential for misrecorded values, clock error readings, etc.

Figure 1 shows two useful plots for monitoring Internet data; one for `DPort` (color changes indicate `DPort` access counts greater than 10, indicative of potentially high traffic on this destination port), and one for source IP address (`SIP`) in the first 10,000 session records (color changes indicate

SIP occurrences of more than 50). Four unusually frequent source IP addresses are immediately evident: 4837, 13626, 33428, and 65246, which occur 371, 422, 479, and 926 times, respectively, in the first 10,000 sessions. The construction of this plot resembles the tracing of a skyline, so Kafadar and Wegman (2006) call it a “skyline plot.” Limits on skyline plots may depend upon time of day, day of week, month, or season.

Another useful display for monitoring session sizes is a streaming control chart, where the statistic that is plotted is a multivariate exponentially-weighted moving average (MEWMA) Hotelling’s T^2 statistic that combines the three transformed ($[\log(1 + \sqrt{x})]$ measures of session size (duration in seconds, number of packets, number of bytes). The parameter for this MEWMA chart, λ , was set at 0.5, in accordance with recommendations in Vardeman and Jobe (1999). Multivariate combinations of features such as Hotelling’s T^2 statistic are useful for detecting small changes in several dimensions but they are less effective than control charts on the individual features if outliers are expected to occur in only one dimension. In this instance of monitoring Internet traffic data, a large session as measured by duration (in seconds) is likely to be large when measured by number of packets or number of bytes, so Hotelling’s T^2 is a sensible statistic to plot on a control chart. Figure 2 shows a static version of an MEWMA plot with smoothing parameter $\lambda = 0.5$ on the last 10,200 observations only. The mean of Hotelling’s T^2 statistic on the entire data set is 39.2, with a standard deviation of 6.05, so a limit at $T^2 = 60$ (3.5 standard deviations: $\Phi(3.5) = 0.99976$) is placed on the control chart to flag rather unusually large sessions based on duration, packets, and bytes. In Figure 2, only 24 out of the 10,200 observations exceed the limit, at more or less random time points, consistent with expectations.

Exploratory data analysis also revealed that scatterplots of the two transformed size variables, $\log(1 + \sqrt{NByte})$ versus $\log(1 + \sqrt{length})$, for a given source IP address, tend to show some correlation but no particular clustering. The top panel of 3 scatterplots in Figure 3 shows three typical source IP addresses: SIP 4837 (which occurred 4,754 times), SIP 13781 (which occurred 1,651 times), and SIP 9675 (which occurred 1,040 times). The remaining six scatterplots in Figure 2 show the scatterplots of these two size variables for six unusual SIP addresses. Source IP 1681 (lower left) indicates 543 sessions that had nearly the same number of bytes transferred (between 22353 and 22385) but the durations of the sessions varied. In fact, all but one of these 543 sessions occurred during the first 23 minutes of the hour. Patterns such as those in Figure 3 could be

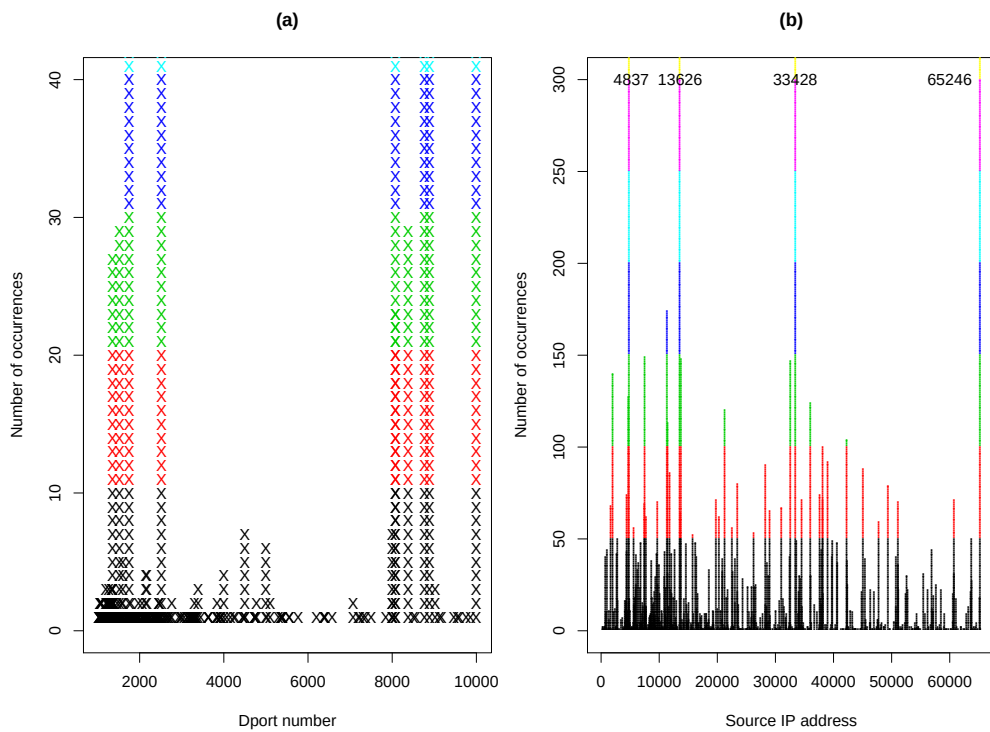


Figure 1: Skyline plots. (a): DPort access; (b): Source IP access

used as “signatures” for source machines, so that a completely different “signature” might signal a potentially attacked machine (i.e., a successful takeover of an internal machine would have a different SIP pattern). This use would require the ability to somehow characterize a plot so that it can be compared with another one; a metric that measures plot similarity or dissimilarity needs to be defined, that would, for example, classify the first two plots in Figure 3 as “similar” (SIPs 4387 and 13781) and the last plot as distinctly different (SIP 23070). From such a metric, groups of SIPs can be defined, and departures from group averages may signal potential attacks. In the same way that residuals from a regression model can indicate important departures and potentially lead to model improvement, what is needed here is the development of methods to “average” similar plots and “subtract” an “historical” plot from an “observed” plot, so that changes in behavior can be readily detected. The dynamic display of plots, such as those shown in Figures 1, 2, and 3, has led Wegman and Marchette (2003) to call them “evolutionary graphical displays.” Many other features of Internet traffic data can be collected (i.e., other information in the TCP/IP headers), which may yield further information useful for detecting potential system attacks.

This research demonstrated the limitations of Tukey’s familiar boxplot display. The boxplot displays the median, fourths (estimates of quartiles), and range of the data, along with “potential outliers.” Designed to “label” roughly 0.7% of outlying observations as “potential outliers” when

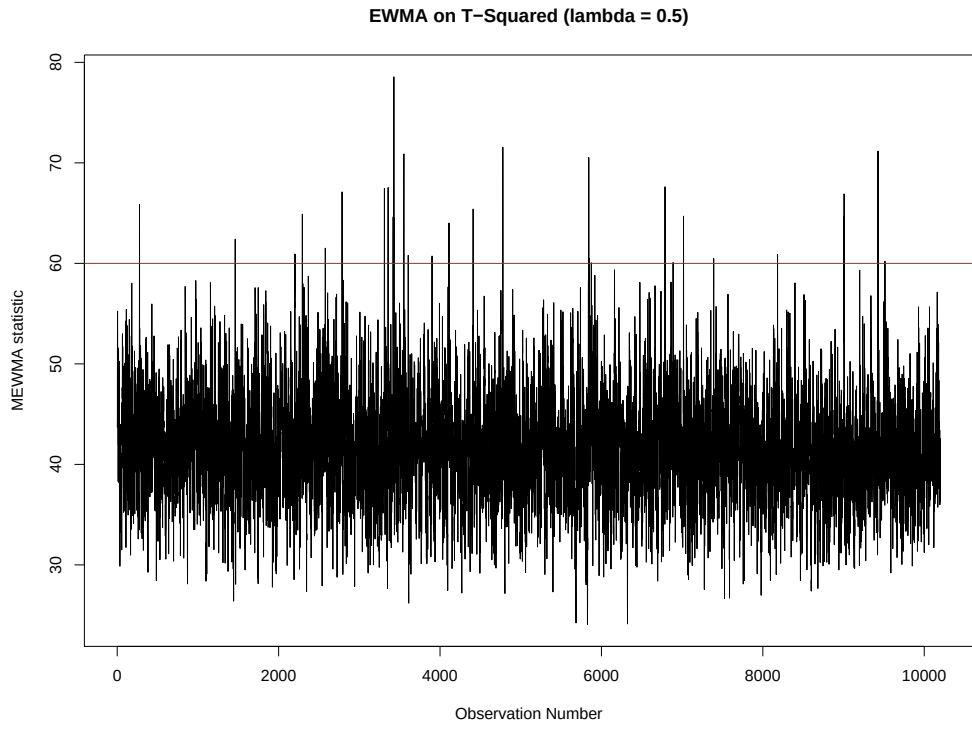


Figure 2: Multivariate EWMA plot of Hotelling's T^2 , last 10,000 values

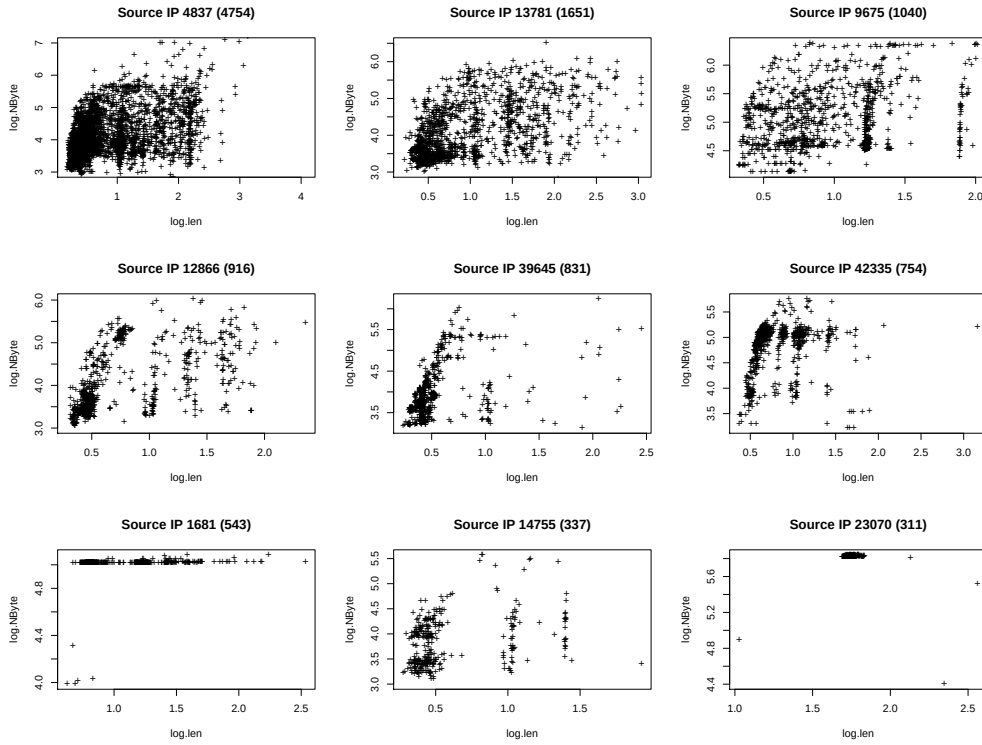


Figure 3: Source IP: log.len vs log.Nbyte

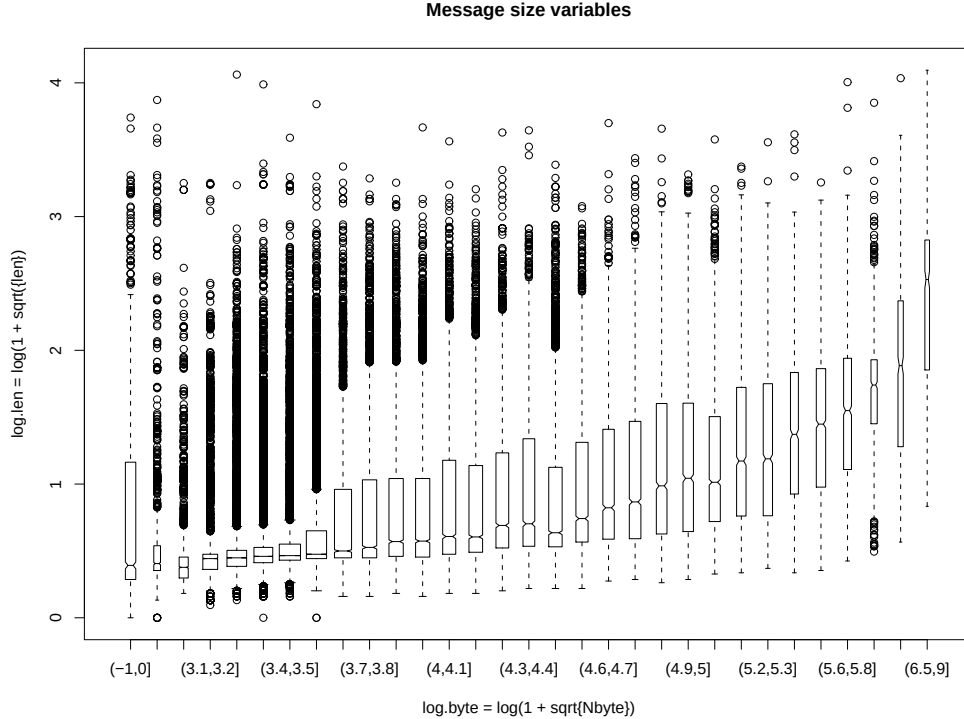


Figure 4: Boxplot of durations of internet session, by category size (number of bytes) of session.

the data come from a Gaussian distribution, 0.7% is a huge fraction when displaying 135,000 observations; see Figure 4. Hofmann, Kafadar, and Wickham proposed an alternative that takes advantage of the huge data set size by estimating quantiles further into the tail. Such estimates are not reliable for small sample sizes, but are more reliable for huge data sets. Quantiles are estimated by letter values (Tukey 1977; Hoaglin, Mosteller, and Tukey 1984). The data displayed with boxplots in Figure 4 are displayed via a letter value display in Figure 5. A manuscript is under revision for publication (Hofmann, Kafadar, Wickham: “Letter value displays”).

3 Forensic Science: Methods and Evaluation

An NRC report was published in 2004 that studied the validity of *compositional analysis of bullet lead* (CABL) (MacFadden et al. (2004), *Weighing the Evidence: Forensic Analysis of Bullet Lead*, National Research Council, The National Academies Press (ISBN 0-309-09079-2): <http://books.nap.edu/catalog>

The P.I. published a paper that discussed matters of data integrity and the scientific method (co-authored with C.S. Spiegelman):

Spiegelman, Clifford H.; Kafadar, Karen: “Data Integrity and the Scientific Method: The Case of Bullet Lead Data as Forensic Evidence (with discussion),” *Chance* 19(2), 17-25 (2006).

Following this report, the National Academies convened a study to identify the needs of the

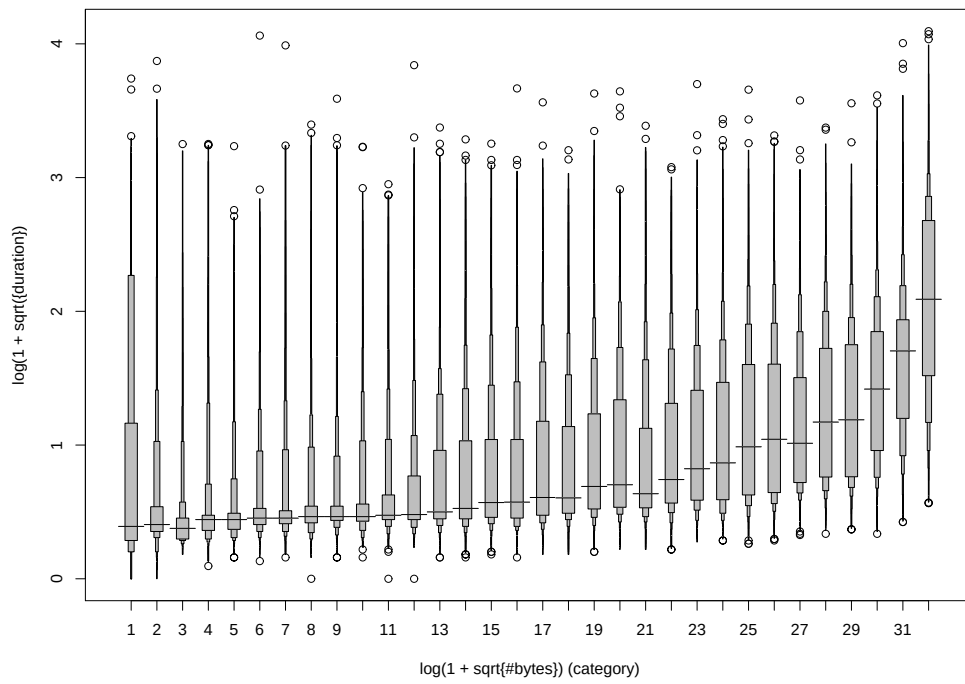


Figure 5: Letter value display of durations of internet session, by category size (number of bytes) of session.

overall forensic science system. This report uncovered a gold mine of opportunities for statistics methodology to be applied in the evaluation of forensic evidence. Some of these issues include:

- Identification of relevant metrics for accuracy and precision
- Design of studies to assess sensitivity and specificity
- Data set size reduction techniques to enhance power
- Prioritization of methods to be studied
- Quality and process monitoring of laboratory procedures
- Criteria for accreditation of laboratories

A report was issued in 2009 that identifies ways to strengthen and enhance our forensic science system:

Edwards, H.T.; Gatsonis, C.; Berger, M.A.; Cecil, J.S.; Denton, M.B.; Fierro, M.F.; Kafadar, K.; Marone, P.M.; Mearns, G.S.; Murch, R.S.; Robertson, C.; Schecter, M.E.; Shaler, R.; Siegel, J.A.; Srihari, S.N.; Wiederhorn, S.M.; Zumwalt, R.E.: *Strengthening Forensic Science in the United*

States: A Path Forward, National Research Council, The National Academies Press (ISBN-10: 0-309-13127-8; ISBN-13: 978-0-309-13127-8), 2009.

(http://books.nap.edu/catalog.php?record_id=12589)

4 High-energy physics

Experimental physicists study the properties, behavior, and rates of reactions among fundamental particles (e.g., leptons such as tau particles, muons, electrons, neutrinos) via experiments designed to accelerate the rate at which reactions occur. Experiments are conducted by accelerating beams of particles through a medium (e.g., electrons through a two-mile tunnel, as at the Stanford Linear Accelerator Center, or through a cyclotron, as at Lawrence Berkeley Laboratory). At the end of the acceleration process is a detector consisting of hundreds of thousands of wires arranged so that each wire will record a voltage if it detects energy (presumably from a particle). Most of these particles fly past one another; experiments are designed to maximize particle collisions and interactions (usually via colliding beams of particles aimed at each other). These collisions are called “events” which are recorded by the data acquisition system, consisting of dozens of computers that record each instance of a “trigger,” or particle that is detected by registering a current in one or more of the wires in the detector. Following the data acquisition stage is the event reconstruction stage, during which hundreds of computer programs aim to reconstruct, as accurately as possible, the momentum, energy, and mass of detected particles at the time of the “trigger” as well as a “nomination” for the type of particle observed and which particles likely came from the same event. Experimental physicists interested in specific particle decay mechanisms. For example, if interest lies in the decay mechanism of the J/ψ particle, they will select events that *appear* to be consistent with current knowledge of this mechanism; if the event includes a particle with a mass that exceeds that of the commonly accepted value of the J/ψ particle, this event would be deemed inconsistent and the data would be excluded from this particular investigation. The goal is to abstract, from the massive data base of events, as many apparent instances of the specific event, which are then used to estimate parameters in a model of its decay process.

Due to the enormous volumes of data that are generated each minute from these events, most of the data are simply ignored. Data are usually selected by censoring rules, called “cuts.” Some

cuts are obvious (e.g., an event whose particles' masses exceed that of the specific particle whose decay reaction is being studied). Other cuts involve the inherent error in the measurement system. For example, if the reaction is known to involve six particles, and the recorded "event" includes nine particles, the experimental physicist is likely to dismiss that event. But if it includes five or seven particles, this event might be retained, on the belief that one of the particles decayed before it could be detected by a wire in the detector, or a particle from a different event was mistakenly included. The "cut" on the number of particles would be 5–7; similar bounds are noted on the other data values that are recorded with each event (e.g., total energy, estimated mass, momentum in the x-, y-, and z-directions for each particle) Each data value is subject to measurement error, including a "nomination" for the type of particle observed based on the its momentum, energy, and mass. A computer applies all of the proposed "cuts" on the variables and returns a file of perhaps only 1000–10,000 events whose particles satisfy the specified constraints. But because the studied reaction is likely to be extremely rare (e.g., estimated frequency of about once a week), this much reduced data includes mostly irrelevant events, called "background" events, from which the "signal" (i.e., data on the relevant events) must be extracted and fitted to the proposed model. (In practice, usually all of the data are fit, and some adjustments are made to "subtract" the effects from the "background" data.)

Historically, experimental physicists have concentrated on the issues of "efficiency" (proportion of events that are truly "signal") and goodness-of-fit measures of the fitted data to the theoretical predictions. Statistical issues include appropriate applications of time series (events may be correlated in time), robust methods (estimating parameters in the presence of contamination), and Bayesian methods (considerable prior information is available). Before that stage, however, are the stages of data acquisition and the methods of "cuts". Presently, experiments are conducted on two-year-old data, due to the time lag between the experiment and the compilation and "censoring" of the data that generated it. It is also believed that thousands of events are censored by the "cuts" and many more thousands are never even considered (dismissed at the first stage as being "uninteresting"). A huge issue is in summarizing the data from experiment in a reliable fashion so that those who might benefit from it can make decisions about its suitability.

Before being able to work on data from particle physics experiments, the P.I. needed to acquire an adequate knowledge of the underlying scientific principles of particle physics theory. To do this,

the P.I. spent nine months in Berkeley with Professor Robert Jacobsen (Department of Physics and Lawrence Berkeley Laboratory). A working paper is under revision for publication in an applied statistics journal (Kafadar, K.; Jacobsen, R.: Statistical analysis of particle physics data, in preparation). The paper provides methods for identifying target events from a massive database of events.

5 Genomics: “Big p, small n”

Studies in genomics involve thousands covariates (gene expressions) on usually only tens or hundreds of observations (DNA samples). The goal of most of these studies is to identify those genes that are expressed in response to a treatment, stimulus, or condition (e.g. diabetes or cancer). This problem involves research into methods for dimension reduction (identifying only the influential covariates) as well as methods for analysis of gene expression data, modeling PCR, and classifying peptides.

Dimension reduction: Penalized Regression Estimators

The problem of accurate and precise estimates of covariance matrices among large numbers of variables leads to the need for dimension reduction methods. Historically, the method of principal components has provided a reduced set of orthogonal variables that are linear combinations of the original variables. These principal components are useful but often not insightful. Alternative methods include modifying the coefficients to “meaningful” values, or penalized regression estimators as a way of shrinking (to zero) the coefficients for potentially insignificant variables. We take the latter approach in this research. This work involved collaborations with Guilherme V. Rocha, and early efforts have been presented at two recent conferences:

- Effect of influential observations on penalized regression estimators, International Conference on Robust Statistics, Prague, 29 Jun 2010.
- Invited presentation, Statistical issues in comparing multidimensional profiles, International Symposium on Business and Industrial Statistics, Portoroz Slovenia, 8 Jul 2010.

This research demonstrates that ordinary penalized regression estimators, such as ridge regression (L_2 loss function: minimize the sum of squared residuals; L_2 penalty function on the

coefficients: sum of the squared coefficients constrained to be less than a pre-selected limit), or Lasso (Tibshirani 1996: L_2 loss function; L_1 penalty function), can be influenced by outliers. A good compromise that pays less attention to outliers, but performs well with both Gaussian and long-tailed (Cauchy) data, combines the use of Lasso's L_1 penalty function with an L_1 loss function. A paper is being prepared that presents the results of this current research, which is on-going.

Analyzing gene expression data: The Square Combining Table

Godfrey (1986) presents a method for obtaining an additive fit to a two-way table called the square combining table. Originally it was proposed as an alternative to median polish (Tukey 1977; Mosteller and Tukey 1977; Hoaglin, Mosteller, and Tukey 1984). Though not as resistant as median polish (which has breakdown equal to one-half of the minimum dimension of the table), it is nonetheless more resistant than ordinary fitting by means (as in classical analysis of variance), can tolerate as much as 20% outliers, and can handle missing data. The method involves taking differences of pairs of columns and pairs of rows, and analyzes the paired-comparisons data. *In fact, gene expression data arise as paired comparisons, so the square combining table is a natural approach to analyzing such data.* This research is being applied to a designed gene experiment currently underway at Indiana University (Andrews lab) and involves G.V. Rocha and R.T. Gutman.

Mathematical formulation of PCR

Gene expression measurements depend on amplification of DNA through a process known as the polymerase chain reaction (PCR). A mathematical model of PCR was developed and validated by experiments in two articles. A third article used PCR data to compare mouse strains. Machine learning methods combined with statistical methods were developed for the classification of peptides in the article by Gehrke et al. (2008).

- Saha, Nilanjan; Watson, Layne T.; Kafadar, Karen; Onufriev, Alexey; Ramakrishnan, Naren; Vasquez-Robinet, Cecilia; Watkinson, Jonathan: "A General Probabilistic Model of the PCR Process," *Applied Mathematics and Computation* 182(1), 232–243 (2006).
- Saha, Nilanjan; Watson, Layne T.; Kafadar, Karen; Ramakrishnan, Naren; Onufriev, Alexey; Rao Mane, Shrinivas; Vasquez-Robinet, Cecilia: "Validation and Estimation of Parameters for a General Probabilistic Model of the PCR Process," *Journal of Computational Biology* 14(1): 97-112 (2007).

- Du, Yunzhi; Davisson, Muriel T.; Kafadar, Karen; Gardiner, Katheleen: “A-to-I pre-mRNA editing of the serotonin 2C receptor: Comparisons among inbred mouse strains,” *Gene* 382: 39–46 (1 Nov 2006).
- Gehrke, Allison; Sun, Shaojun; Kurgan, Lukasz A.; Ahn, Natalie G.; “Improved machine learning methods for analysis of gas phase chemistry of peptides,” *Bioinformatics* 9:515; doi:10.1186/1471-2105-9-515, 2008.

6 Additional research: Length Biased Sampling and Library Search

Length biased sampling

Data that are collected from any type of measurement system may be subjected to various types of bias, such as selection bias, observation bias, etc. Some of these biases were discussed in the P.I.’s co-authored report of NASA’s National Aviation Operations Monitoring Service (Nair et al. 2009). An important, and often overlooked, bias arises when the size of the data value itself increases the probability of the observation. This situation is known as length-biased sampling. It arises when larger particles are more likely to be observed than smaller ones, or when longer durations are more likely to be caught by the measurement process than shorter ones. In randomized cancer screening trials, slower-growing disease that has a long pre-clinical duration is more likely to be captured by a screening modality (e.g., mammography or PSA) than disease with short pre-clinical duration. Length biased sampling influences the evaluation of screening: long pre-clinical duration is often positively correlated with long clinical duration, and hence screen-detected cases will appear to live longer (longer clinical durations) than non-screen-detected cases, even after having accounted for lead time bias.

The effect of length biased sampling on the assessment of benefit (survival time) in randomized cancer screening trials was studied in Kafadar and Prorok (2009):

Kafadar, K.; Prorok, P.C.: “Effect of length-biased sampled sojourn times on the survival distribution in randomized cancer screening trials,” *Statistics in Medicine* 28:2116-2146, 2009.

In situations where pre-clinical and clinical durations are highly correlated, the effect can be as large as 20-30%; i.e., if the “apparent” benefit of screening is extended survival by one year, 20-30% of that benefit is due simply to the length-biased sampling. This research has consequences

for many studies where the probability of observing the data depends on its size (length, volume, etc.) and can influence inferences when data on smaller sizes are ignored (e.g., less frequent but highly influential events).

Library Search

Length-biased sampling also arises in connection with the retrieval of library records, resulting in missed references in common search engines. These issues were explored through designed studies in library research:

- Beall, Jeffrey; Kafadar, K.: The effectiveness of copy cataloging at eliminating typographical errors in shared bibliographic records, *Library Resources & Technical Services* 48(2): 92–101 (April 2004).
- Beall, Jeffrey; Kafadar, Karen: The Proportion of NUC Pre-56 Titles Represented in OCLC WorldCat, *College & Research Libraries* 66(5): 431–435 (2005).
- Beall, Jeffrey; Kafadar, Karen: Measuring Typographical Errors’ Impact on Retrieval in Bibliographic Databases (invited), *Cataloging & Classification Quarterly* 44(3/4): 197–211 (2007).
- Beall, Jeffrey; Kafadar, Karen: Measuring the Extent of the Synonym Problem in Full-text Searching, *Evidence Based Library and Information Practice* 2008 3(4), 18–33.

7 Impact

The impact of this research has been the development of methods for analysis and display of massive data. A series of issues were studied: graphical methods (letter value plots), dimension reduction, evaluation of forensic science methods, analysis of gene expression data, and effects of length biased sampling. Correct inferences from data depend critically on appropriate methods for analysis. As a result of this research, better methods for analyzing massive data have been developed and demonstrated on data from diverse contexts, including genomics, imaging, forensics, text search, internet communications, medical screening trials, and high-energy particle physics. All have important implications in the understanding of data related to national security.

The research from this grant has been posted at <http://mypage.iu.edu/~kkafadar>.

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