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MMDS 2008: Algorithmic and Statistical Challenges in Modern Large-Scale Data Analysis, Part I

By Michael W. Mahoney, Lek-Heng Lim, and Gunnar E. Carlsson

The 2008 Workshop on Algorithms for Modern Massive Data Sets (MMDS 2008), held at Stanford University, June 25–28, had two goals: first, to explore novel techniques for modeling and analyzing massive, high-dimensional, and nonlinearly structured scientific and Internet data sets, and second, to bring together computer scientists, statisticians, mathematicians, and data analysis practitioners to promote the cross-fertilization of ideas. The workshop was sponsored by NSF, DARPA, Yahoo! and LinkedIn.

MMDS 2008 grew out of discussions of our vision for what the algorithmic, mathematical, and statistical analyses of large-scale, complex data sets should look like a generation from now. These discussions occurred in the wake of MMDS 2006, which had been motivated by the complementary perspectives brought by the numerical linear algebra and theoretical computer science communities to combinatorial, numerical, and randomized algorithms in modern informatics applications (see www.siam.org/news/news.php?id=1019). As with the 2006 meeting, the MMDS 2008 program was intensely interdisciplinary, with close to 300 participants representing a wide spectrum of research in modern large-scale data analysis.

Diverse Approaches to Modern Data Problems

A common way to model a large social or information network is with an *interaction graph model* $G = (V,E)$, in which nodes in the vertex set V represent "entities" and the edges (whether directed or undirected, weighted or unweighted) in the edge set E represent "interactions" between pairs of entities. Alternatively, because an $m \times n$ real-valued matrix A provides a natural structure for encoding information about m objects, each described by n features, these and other data sets can be modeled as matrices. Because of their large size, their extreme sparsity, and their complex and often adversarial noise properties, data graphs and data matrices arising in modern informatics applications present considerable challenges and opportunities for interdisciplinary research. These algorithmic, statistical, and mathematical challenges were the focus of MMDS 2008.

Historically, very different perspectives have been brought to such problems. Computer scientists interested in data mining and knowledge discovery commonly view the data in a database as an accounting or a record of everything that happened in a particular setting. The database might consist of all customer transactions over the course of a month, or of all friendship links between members of a social networking site. From this perspective, the goal is to tabulate and process the data at hand to find interesting patterns, rules, and associations. An example of an association rule is the proverbial "People who buy beer between 5 PM and 7 PM buy diapers at the same time." The performance or quality of such a rule is judged by the fraction of the database that satisfies the rule exactly, and the problem then boils down to that of finding frequent item sets. This is a computationally hard problem, and much algorithmic work has been devoted to its exact or approximate solution under different models of data access.

When it comes to Web-scale data analysis, an algorithm that is expensive in floating-point cost but readily parallelizable is often a better choice than a less expensive algorithm that is not parallelizable.

A very different way to view the data, more common among statisticians, is as a particular random instantiation of an underlying process describing unobserved patterns in the world. In this case, the goal is to extract information about the world from the noisy or uncertain data that is observed. To achieve this, one might posit the model $data \sim F_\theta$ and $\text{mean}(data) = g(\theta)$, where F_θ is a distribution that describes the random variability of the data around the deterministic model $g(\theta)$ of the data. Using this model, researchers would analyze the data to make inferences about the underlying processes and predictions about future observations. From this perspective, modeling the noise component or variability is as important as modeling the mean structure, in large part because understanding the former is necessary for understanding the quality of the predictions made. This approach even permits predictions about events not observed before—it is possible to give, for example, the probability that a given user on a given Web site will click on a given advertisement presented at a given time of day, even if this particular event does not exist in the database.

Of course, we have many indications that the two perspectives are not incompatible: Statistical and probabilistic ideas are central to many recent efforts to develop improved approximation algorithms for matrix problems; otherwise-intractable optimization problems on graphs and networks yield to approximation algorithms when assumptions are made about the network participants; much recent work in machine learning draws on ideas from both areas; and in boosting, a statistical technique that fits an additive model by minimizing an objective function with a method like gradient descent, the computation parameter, i.e., the number of iterations, also serves as a regularization parameter.

Given the diversity of possible perspectives, MMDS 2008 was loosely organized around six hour-long tutorials that introduced participants to the major themes of the workshop; each is briefly summarized either here or in Part II of this article.

Large-Scale Informatics: Problems, Methods, and Models

Christos Faloutsos of Carnegie Mellon University opened the tutorial "Graph Mining: Laws, Generators and Tools" by describing a wide range of applications in which graphs arise naturally. Large graphs that arise in modern informatics applications, he pointed out, have structural properties very different from those of traditional Erdős–Rényi random graphs; an example is the heavy-tailed behavior of degree distributions, eigenvalue distributions, and other statistics that result from subtle correlations.

These structural properties have been studied extensively in recent years and have been used to develop numerous well-publicized models; Faloutsos also described empirically observed properties that are not well reproduced by existing models. Most models, for example, predict that over time a graph should become sparser and the diameter should grow as $O(\log N)$, or perhaps $O(\log \log N)$, where N is the number of nodes at the current timestep; empirically, though, many of these networks have been observed to densify over time and to shrink in diameter. To explain these phenomena, Faloutsos described a model based on Kronecker products and another in which edges are added via an iterative "forest fire" mechanism. With appropriate choice of parameters, both models can be made to reproduce a range of static and dynamic properties much wider than those of previous generative models.

Building on this modeling foundation, Faloutsos described several graph-mining applications of current interest: methods for finding nodes that are central to a group of individuals; use of the singular value decomposition and recently developed tensor methods to identify anomalous patterns in time-evolving graphs; modeling information cascades in the blogosphere as virus propagation; and novel methods for fraud detection.

Other developments in Web-scale data analysis were the subject of Edward Chang's tutorial, "Mining Large-scale Social Networks: Challenges and Scalable Solutions." After reviewing emerging applications—such as social network analysis and personalized information retrieval—that have arisen as we transition from Web 1.0 (links between pages and documents) to Web 2.0 (links between documents, people, and social platforms), Chang, of Google Research, covered four applications in detail: spectral clustering for network analysis, frequent-itemset mining, combinatorial collaborative filtering, and parallel support vector machines (SVMs) for personalized search. In all these cases, he emphasized, the main performance requirements are "scalability, scalability, scalability."

Modern informatics applications like Web search afford easy parallelization—for example, the overall index can be partitioned in such a way that even a single query can use multiple processors. Moreover, the peak performance of a machine is less important than the price–performance ratio. In this environment, scaling up to petabyte-sized data often means working in a software framework that, like MapReduce or Hadoop, supports data-intensive distributed computations running on large clusters of hundreds, thousands, or even hundreds of thousands of commodity computers. This differs substantially from the scalability issues that arise in traditional applications of interest in scientific computing. A recurrent theme in Chang's presentation was that an algorithm that is expensive in floating-point cost but readily parallelizable is often a better choice than a less expensive algorithm that is not parallelizable.

As an example, Chang considered SVMs: Although widely used, mainly because of their empirical success and attractive theoretical foundations, they suffer from well-known scalability problems in both memory use and computational time. Chang described a parallel SVM algorithm that addresses these problems—it reduces memory requirements by performing a *row-based* incomplete Cholesky factorization (ICF) and by loading only essential data to each of the parallel machines, and it reduces computation time by intelligently reordering computational steps and performing them on parallel machines. The traditional *column-based* ICF, he pointed out, is better in a single-machine setting but is not suitable for parallelization across many machines.

Part II of this article will appear in an upcoming issue of SIAM News.

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MMDS 2008: Algorithmic and Statistical Challenges in Modern Large-Scale Data Analysis, Part II

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By Michael W. Mahoney, Lek-Heng Lim, and Gunnar E. Carlsson

Algorithmic Approaches to Networked Data

In an algorithmic perspective on improved models for data, Milena Mihail of the Georgia Institute of Technology began by describing the recent development of a rich theory of power-law random graphs, i.e., graphs that are random conditioned on a specified input power-law degree distribution. With the increasingly wide range of large-scale social and information networks now available, however, generative models that are structurally or syntactically more flexible have become necessary. Mihail described two such extensions: one in which semantics on nodes is modeled by a feature vector, with edges added between nodes based on their semantic proximity, and another in which the phenomenon of associativity/disassociativity is modeled by fixing the probability that nodes of a given degree d_i tend to link to nodes of degree d_j.

A small extension in the parameters of a generative model, of course, can lead to a large increase in the observed properties of generated graphs. This observation raises interesting statistical questions about model overfitting, and argues for more refined and systematic methods for model parameterization. It also leads to some of the new algorithmic questions that were the topic of Mihail's talk.

Mihail posed the following algorithmic problem for the basic power-law random graph model: Given as input an N-vector specifying a degree sequence, determine whether a graph with that degree sequence exists and, if it does, efficiently generate one (perhaps approximately uniformly randomly from the ensemble of such graphs). Such realizability problems have a long history in graph theory and theoretical computer science. Because their solutions are intimately related to the theory of graph matchings, many generalizations of the basic problem can be addressed in a strict theoretical framework. For example, motivated by associative/disassociative networks, Mihail described recent progress on the joint-degree matrix realization problem: Given a partition of the node set into classes of vertices of the same degree, a vector specifying the degree of each class, and a matrix specifying the number of edges between any two classes, determine whether such a graph exists and, if it does, construct one. She also described extensions of this basic problem to connected graphs, to finding minimum cost realizations, and to finding a random graph satisfying those basic constraints.

The Geometric Perspective: Qualitative Analysis of Data

Gunnar Carlsson of Stanford University offered an overview of geometric and topological approaches to data analysis, which seek to provide insight into data by imposing a geometry on it. In certain applications, such as physics, the phenomena studied support clean explanatory theories that indicate exactly what metric to use to measure the distance between pairs of data points. This is not the case in most MMDS applications. It is not obvious, for instance, that the Euclidean distance between DNA expression profiles in high-throughput microarray experiments captures a meaningful notion of distance between genes. Similarly, despite the natural geodesic distance associated with any graph, the sparsity and noise properties of social and information networks mean that in practice this is not a particularly robust notion of distance.

Part of the problem is thus to define useful metrics—especially because certain applications, including clustering, classification, and regression, often depend sensitively on the choice of metric. Recently, two design goals have emerged. First, don't trust large distances; because distances are often constructed from a similarity measure, small distances reliably represent similarity, but large distances make little sense. Second, trust small distances only a bit—after all, similarity measurements are still very noisy. These ideas are the basis for much work on Laplacian-based nonlinear dimension reduction, i.e., manifold-based methods currently popular in harmonic analysis and machine learning. More generally, the ideas suggest the design of analysis tools that are robust to stretching and shrinking of the underlying metric, particularly in applications like visualization, in which qualitative properties, such as how data is organized on a large scale, are of interest.

Much of Carlsson's tutorial was devoted to these analysis tools and their application to natural image statistics and data visualization. Homology, the crudest measure of topological properties, captures such information as the number of connected components or the presence of holes of various dimensions in the data. Importantly, although the computation of homology is not feasible for general topological spaces, the space can often be modeled in terms of simplicial complexes, in which case the computation of homology boils down to the linear algebraic computation of the Smith normal form of certain data-dependent matrices.

Carlsson also described persistent homology, an extension of the basic idea in which some parameters, such as the number of nearest neighbors and error parameters, can be varied. A "bar code signature" can then be associated with the data set. Long segments in the bar code indicate the presence of a homology class that persists over a long range of parameter values. This can often be interpreted as corresponding to large-scale geometric features in the data; shorter segments can be interpreted as noise.

Statistical and Machine Learning Perspectives

Given a set of measured values of attributes of an object $\mathbf{x} = (x_1, x_2, \ldots, x_n)$, the basic predictive or machine learning problem is to predict or estimate the unknown value of another attribute y. The quantity y is the "output" or "response" variable, and $\{x_1, x_2, \ldots, x_n\}$ are the "input" or "predictor" variables. In regression problems, y is a real number; in classification problems, y is a member of a discrete set of unorderable categorical values (such as class labels). In either case, this can be viewed as a function estimation problem—the prediction takes the form of a function $\hat{y} = F(\mathbf{x})$ that maps a point $\mathbf{x}$ in the space of all joint values of the predictor variables to a point $\hat{y}$ in the space of response variables, and

the goal is to produce an $F(\cdot)$ that minimizes a loss criterion.

Jerome Friedman of Stanford University opened the tutorial "Fast Sparse Regression and Classification" by pointing out that it is common to assume a linear model, in which $F(\mathbf{x}) = \sum_{j=1}^{n} a_j x_j$ is modeled as a linear combination of the n basis functions. Unless the number of observations is much, much larger than n, however, empirical estimates of the loss function exhibit high variance. To make the estimates more regular, one typically considers a constrained or penalized optimization problem

$$\hat{\mathbf{a}}(\lambda) = \text{argmin}_{\mathbf{a}} \hat{L}(\mathbf{a}) + \lambda P_{\gamma}(\mathbf{a}),$$

where $\hat{L}(\cdot)$ is the empirical loss and $P_{\gamma}(\cdot)$ is a penalty term. The choice of an appropriate value for the regularization parameter λ is a classic model selection problem, for which cross validation can be used. The choice for the penalty depends on what is known or assumed about the problem at hand. A common choice is $P_{\gamma}(\mathbf{a}) = \|\mathbf{a}\|_{\gamma}^{\gamma} = \sum_{j=1}^{n} |a_j|^{\gamma}$. This interpolates between the subset selection problem ($\gamma = 0$) and ridge regression ($\gamma = 2$) and includes the well-studied lasso ($\gamma = 1$). For $\gamma \leq 1$, sparse solutions (which are of interest due to parsimony and interpretability) are obtained, and for $\gamma \geq 1$, the penalty is convex.

Choice of an optimal (λ,γ) by cross validation, although possible, can be prohibitively expensive even when the loss and penalty are convex, because of the need to perform computations at a large number of discretized pairs. Path-seeking methods have been studied for this situation. Consider the path of optimal solutions $\{\hat{\mathbf{a}}(\lambda) : 0 \leq \lambda \leq \infty\}$, which is a one-dimensional curve in the parameter space $\mathbb{R}^n$. If the loss function is quadratic and the penalty function is piecewise linear, as with the lasso, then the path of optimal solutions is piecewise linear and homotopy methods can be used to generate the full path in time not much greater than that needed to fit a single model at a single parameter value. Friedman described a generalized path-seeking algorithm that solves this problem for a much wider range of loss and penalty functions (including some nonconvex functions) very efficiently.

In a tutorial titled "Kernel-based Contrast Functions for Sufficient Dimension Reduc-tion," Michael Jordan of the University of California, Berkeley, considered the dimension reduction problem in a supervised learning setting. Such methods as principal components analysis, Johnson–Lindenstrauss techniques, and recently developed Laplacian-based nonlinear methods are often used but have limited applicability—for example, the axes of maximal discrimination between the two classes may not align well with the axes of maximum variance. The hope is that there exists a low-dimensional subspace S of the input space X that can be found efficiently and that retains the statistical relation between X and the response space Y. Conventional approaches to this problem of sufficient dimension reduction make strong modeling assumptions about the distribution of the covariate X and/or the response Y. Jordan considered a semiparametric formulation, in which the conditional distribution $p(Y \mid X)$ is treated nonparametrically and the goal is to estimate the parameter S. He showed that this problem can be formulated in terms of conditional independence and evaluated in terms of operators on reproducing kernel Hilbert spaces (RKHSs).

Claims about the independence of two random variables can be reduced to claims about correlations between them when transformations of the random variables are considered: that is, X_1 and X_2 are independent if and only if

$$\max_{h_1, h_2 \in \mathcal{H}} \text{Corr}(h_1(X_1), h_2(X_2)) = 0$$

for a suitably rich function space $\mathcal{H}$. If $\mathcal{H}$ is L_2 and thus contains the Fourier basis, this reduces to a well-known fact about characteristic functions. More interesting from a computational perspective—given that by the "reproducing" property, function evaluation in an RKHS reduces to an inner product—this also holds for suitably rich RKHSs. This use of RKHS ideas to solve the sufficient dimension reduction problem cannot be viewed as a kernelization of an underlying linear algorithm, as is typically the case when such ideas are used (e.g., with support vector machines) to provide basis expansions for regression and classification. Rather, this is an example of how RKHS ideas provide algorithmically efficient machinery for optimizing a much wider range of statistical functionals of interest.

Conclusions and Future Directions

Along with the topics presented in the tutorials, participants heard about a wide variety of data applications: to movie and product recommendations, predictive indexing for fast Web search, pathway analysis in biomolecular folding, functional MRI, high-resolution terrain analysis, galaxy classification, and other applications in computational geometry, computer graphics, computer vision, and manifold learning. We heard about a novel use of approximation algorithms to probe the community structure of large social and information networks as a way to test the claim that such data are even consistent with the manifold hypothesis (which they clearly are not). In all these cases, scalability was a central issue—motivating discussion of external memory algorithms, novel computational paradigms like MapReduce, and communication-efficient linear algebra algorithms. Interested readers are invited to visit the conference Web site, http://mmds.stanford.edu.

The feedback we received made it clear that MMDS has struck a strong interdisciplinary chord. Thinking ahead to a future MMDS workshop, nearly every statistician we spoke with hoped to see more statisticians; nearly every researcher in scientific computing hoped for more data-intensive scientific computation. Practitioners from application domains called for more applications, and just about every theoretical computer scientist expressed the hope for more of the same. MMDS is generating interest as a developing interdisciplinary research area at the interface between computer science, statistics, applied mathematics, and scientific and Internet data applications.

Keep an eye out for future MMDS workshops!

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