Data Mining
Tools for Exploring Big Data

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Modern data mining combines familiar and novel statistical methods to identify reproducible patterns in big data. The objective outcome is prediction. If your model predicts new data better than alternatives, then you’ve made a contribution. Rather than build a model that relates one or two experimental results to a response, data mining involves searching for patterns. Such searches commonly scan thousands of features, looking for the few that are predictive of the response. The search might be entirely automated or allow expert insight. Once considered vile, data mining has become respectable, useful, and necessary. Data mining is needed when dealing with wide data tables, those having more variables than cases.

These lectures introduce data mining through a combination of lectures and examples. You’ll see examples that look for patterns in voting behavior, patients at risk of a disease, prospective job candidates, and credit applications that reveal fraud. In each illustration, the goal is prediction. Rather than interpret a pattern found in one set of data, the objective is to predict new data. Interpretation is fun, but we’ll exercise considerable restraint to avoid confusing association with causation. Even if you stick to simple models, concepts from data mining can diagnose if you’ve missed an important feature of your data.

Data mining does not require exotic hardware or software. Today’s PC would have been a supercomputer in 1999. You can explore large datasets quite well with nothing more than regression and a laptop. Once we develop the fundamentals, you’ll be able to appreciate the strengths and weaknesses of exotic methods. The course begins with regression, then covers logistic regression, neural networks, and classification and regression trees, with a bit of cluster analysis.

You need to do data mining to learn data mining. For this class, we’ll use a combination of R and JMP from SAS. JMP interactively handles large data sets and includes an extensive collection of algorithms for building and assessing models. The software is highly interactive with amazing interactive graphics. Two class sessions are devoted to lab time so that you can try some of these tools yourself in a supervised lab.

Participants who attend these lectures are encouraged to work on a project associated with an ICPSR data set. The work on that project will help you learn how the tools work. Possible topics for this project include data from studies related to elections, health outcomes, criminal sentencing, economics, and social activities.
Guide to Planned Lectures

Lecture 1. Introduction, Exploring Large Data Sets

Good data analysis begins by looking at the data. That can be hard to do when the dataset has hundreds of columns, but it’s not impossible. This lecture introduces data mining and explores several datasets using interactive graphics, a key strength of JMP. The objectives are to gain familiarity with the data, spot unusual patterns, recognize collinear variables, and form conjectures. Hypothesis generation, not just testing, is an important aspect of data mining.

Predictive models aim to predict or classify new observations. Regression analysis is the most commonly used predictive methodology in statistics and the benchmark for data mining as well. Much of the success that you can have with a regression model comes from the fact that regression comes with well-developed diagnostics combined with tools for inference that can be enhanced with bootstrap resampling.

A key challenge in data mining is finding the right set of explanatory variables. We may start from those that come in the data directly, but we usually need to expand this set. Even though we may start with a wide data set, the columns in the data may not be the right ones to use in a data mining analysis. The simplest extensions are interactions, products of the original explanatory variables. Graphical tools known as profilers help us explore the structure of models, helping convey the impact of interactions and nonlinearity. Before we can exploit interactions in data mining, we need to be acquainted with what they are and what they do in a model.

Calibration is an important additional diagnostic of the performance of a model, one that is easy to check and useful in applications. In many cases, such as when building models for a 0/1 response, it is far easier to calibrate the original regression model rather than switch to a more elaborate method. This lecture will also introduce some of the data sets used in the class, particularly data from the 2008 US presidential election.

Lecture 2. Data Mining with Regression

Wide data sets challenge the thoughtful modeler. Even the best researcher with a clear theory will wonder if other variables might be predictive of the response. Since most collections of possible explanatory variables are highly correlated, it can be very hard (and risky) to impose a strong interpretation on the estimates. That’s where methods that automatically search for predictors (explanatory variables that don’t really explain but do predict the response) become necessary. The best known, most disparaged, and yet perhaps most useful is the greedy search provided by stepwise regression. Even if you have your heart set on one of the new algorithms, you should always set a baseline for comparison with stepwise regression.

Most datasets contain missing values, and this class discusses simple methods for handling these anomalies – that are far too common – when data mining. We’ll also borrow ideas from multivariate analysis (e.g., principal components and cluster analysis) to find interesting views of data.

Lecture 3. Model Validation

Automated searches for patterns increase the risk of over-fitting, adding variables to a predictive model that are not in fact predictive. Over-fitting is common; we’ve all seen applications in which a model fits the observed sample well but predicts new data poorly. This lecture considers how to control stepwise regression. Cross-validation and the roughly equivalent criterion known
as AIC are often recommended, but we’ll come down on the side of methods related to the
Bonferroni criterion.

Cross-validation is often used more generally to pick a model. An important example of this use
of cross-validation comes in picking the best model offered by the lasso, a different way of
picking the variables for a model that shrinks the model estimates. Though handy, cross-
validation has problems, too. We’ll identify situations when it works and others that lead to
problems.

Lecture 4. Holiday

July 4th.

Lecture 5. Lab Session

Hands on time in the Michigan Lab.

Lecture 6. Logistic Regression and Classification

Many modeling tasks seek to predict qualitative behavior, such as whether a voter participates in
an election or a customer makes a purchase. Models for choices – classifiers – require different
methods that adjust for the categorical nature of the response. The canonical example is logistic
regression for a binary response. Calibration remains important, and a calibrated linear
regression often matches well to a logistic regression. That’s good, because searching for the
best logistic regression can be very slow!

Changing the response from numerical to categorical also changes the way that we measure how
well a model performs. Least squares may be reasonable, but other metrics such as ROC curves
and confusion matrices are popular.

Lecture 7. Neural Networks and Boosting

Regression models produce an equation that “explains” how the model predicts new cases.
Alternative methods such as neural networks work differently. Neural networks, and the closely
related method known as projection pursuit regression, blend several regression models together
using heuristics borrowed from engineering and biology. Model visualization – profiling –
becomes necessary for understanding what a network does.

Boosting is a general-purpose technique for improving – boosting – the performance of a model.
Boosted networks are an example of model averaging in which you combine several different
models to arrive at a prediction (another is known as bagging). We’ll explore boosting in the
context of neural networks, but you should recognize that it can be used effectively in many
other situations.

Lecture 8. Classification and Regression Trees, Random Forests

Regression trees (a.k.a., CART with the closely related classification trees) are different enough
from regression models that they deserve more time to appreciate. In place of an equation, a tree
produces a set of rules that determine how to predict or classify the response. This lecture uses
trees as alternatives to regression models, considering what they are very good at (e.g., finding
interactions and producing a set of rules that is often more appealing than the concept of an
equation) and what they don’t do so well (e.g., smooth patterns). Part of the appeal of using trees is the elegant implementation in JMP.

Trees are neat, but if you like them, you’ll want to learn how to grow forests. Random forests are another example of mode averaging. Random forests use bootstrap resampling to create multiple data sets that can be used to fit alternative models. Averaging the predictions of these models usually produces a better prediction than any one model alone. The ideas apply widely beyond trees to virtually any predictive model.

Lecture 9. Lab Session

Hands on time in the Michigan Lab.

Lecture 10. Further Topics and Comparisons

We’ll use this last class to review prior topics and to handle the inevitable overflow from prior lectures. We’ll also discuss an ongoing project that applies regression to text mining: modeling text rather than numbers. Once you see how that’s done, you’ll see how to expand the scope of models to images and other types of novel data.

Time permitting, we will take a look at methods for very large data sets based on ideas known as kernels and random projection. These ideas have produced a wave of techniques related to principal component regression that can be used when dealing with millions of variables.
References

If you would like to do some reading to accompany these lectures, or perhaps follow up afterwards, here are a few papers, books, and web sites that you might find useful.

Berk starts from the regression point of view and includes trees and ensemble methods like bagging and random forests. There’s also a bit on smoothing via regression.

This paper describes ensemble methods like bagging using the example of random forests. There are examples with cross-validation as well.

Statistics missed the boat, sticking to asymptotic estimates for small samples as the world of computing and large data bases exploded. Several good discussions accompany this article.

This classic popularized the use of tree-based models and the use of cross-validation in picking good models. Still a good read.

Over-fitting is a serious problem when the data suggest the model, often leading to wildly optimistic promises of prediction accuracy.

Using 3,000,000 months of credit card activity and 67,000 possible features, we show how to use least squares regression to build a model that predicts as well (or better) than the computational learning algorithm known as C4.5. The algorithm is now implemented in the SAS enterprise miner software package.

This paper shows how to use a theory to guide the allocation of the chance for false positives over a sequence of tests, as in the case of stepwise regression.

Jerry Friedman is one of the most creative modelers in statistics. Here’s his take on how statistics can play a more central role in a world of large data sets.

This paper shows that nonparametric regression can be viewed as a special case of stepwise regression. It’s all in the choice of the \(x\) variables that the search considers.

There are a lot of books on data mining, but most talk more about assembling the data and are written for computer science. Assembling the data is a hard part of the problem, and if you get it wrong, it does not matter how you do the modeling. This book describes some of those issues, but goes on to summarize the statistical methods as well. A nice high-level view of models and patterns in general.


If my predictions are more accurate than yours, I profit and you lose. It’s no wonder that data mining has become important in the business world. Be they pharmaceuticals like Merck and Pfizer or web sellers like Amazon, a large chunk of the value of many firms lies in their proprietary data.


Much of the initial development of methods for handling large data sets began outside of statistics, in an area known as computational learning or, more boldly, knowledge discovery. Computer science was quick to see the importance of getting value from large databases, and forged ahead. They certainly came up with better names (e.g., neural network versus projection pursuit regression). You can download this book online for free.


Emphasizes role in business decision making, with 100+ pages introducing the role of data mining. Wide scope of methods with discussion of presentation, communication of results, and privacy issues.


This text introduces many of the principles that guide modern research on modeling within computer science, nicely called “machine learning.” The text introduces the foundations by developing the connection between statistics and information theory. These connections provide heuristics for the computing algorithms.


You have to think about the scope of the search when you build a model by finding the best fit possible using anything from a wide database. Information theory (ideas that show how to fit more data on your computer disk or make cellular telephones work) turns out to offer a very useful paradigm for judging models.


This is a wide-reaching, medium-level math introduction. The presentation is not nearly so technical as Hastie. It includes many of the ideas that are now used in computer science for modeling, such as the so-called kernel trick and support vector machines. (It has little discussion of regression or logistic regression.)


Introduces data mining and R five case studies, but some of the data is really small (like $n = 7$). Examples include nature, stock trading, fraud detection, and microarrays. The methods include the usual ones (like regression), but reach out to support vector machines (SVM) and multivariate adaptive regression splines (MARS).

The emphasis here is on trees and association rules. The coverage is terse, but comprehensive with much of the terminology mentioned. Technical material is included, but confined to boxes. The examples are closely tied to the WEKA software tools. Examples use small data sets.

www.kdnuggets.com

This web site links to software, data and conferences, including the data sets used for its annual competitions to see what sort of data mining software can predict a hold-back sample the best.