The Interrelationship Between Physics, Mathematics and Chemistry - A Study

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Abstract

This paper studies the relationship between mathematics and physics has been a subject of study of mathematicians and physicists since Antiquity, and more recently also by historians and educators. Mathematical science, Physics, and chemistry has had long expansion. This expansion has been ongoing for decades, but it has accelerated greatly over the past 10-20 years. Some of these links develop naturally, because so much of science and engineering now builds on computation and simulation for which the mathematical sciences are the natural language. In addition, data-collection capabilities have expanded enormously and continue to do so, and the mathematical sciences are innately involved in distilling knowledge from all those data. However, mechanisms to facilitate linkages between mathematical scientists and researchers in other disciplines must be improved.

The impacts of mathematical science research can spread very in some cases, because a new insight can quickly be embodied in software without the extensive translation steps that exist between, say, basic research in chemistry and the use of an approved pharmaceutical. When mathematical sciences research produces a new way to compress or analyze data, value financial products, process a signal from a medical device or military system, or solve the equations behind an engineering simulation, the benefit can be realized quickly. For that reason, even government agencies or industrial sectors that seem disconnected from the mathematical sciences have a vested interest in the maintance of a strong mathematical sciences enterprise for our nation. And because that enterprise must be healthy in order to contribute to the supply of well-trained individuals in science, technology, engineering, and mathematical (STEM) fields, it is clear that everyone should care about the vitality of the mathematical sciences.

This chapter discusses how increasing interaction with other fields has broadened the definition of the mathematical sciences. It then documents the importance of the mathematical sciences to a multiplicity of fields. In many cases, it is possible to illustrate this importance by looking at major studies by the disciplines themselves, which often list problems with a large mathematical sciences component as being among their highest priorities.

Key words: science, technology, engineering, physics, mathematical sciences, mathematical (STEM) fields.

Introduction

Over the past decade or more, there has been a rapid increase in the number of ways the mathematical sciences are used and the types of mathematical ideas being applied. Because many of these growth areas are fostered by the explosion in capabilities for simulation, computation, and data analysis (itself driven by orders-of-magnitude increases in data collection), the related research and its practitioners are often assumed to fall within the umbrella of computer science. But in fact people with varied backgrounds contribute to this work. The process of simulation-based science and engineering is inherently very mathematical, demanding advances in mathematical structures that enable modeling; in algorithm development; in fundamental questions of computing; and in model validation, uncertainty quantification, analysis, and optimization. Advances in these areas are essential as computational scientists and engineers tackle greater complexity and exploit advanced computing. These mathematical science aspects demand considerable intellectual depth and are inherently interesting for the mathematical sciences.

At present, much of the work in these growth areas—for example, bioinformatics, Web-based companies, financial engineering, data analytics, computational science, and engineering—is handled primarily by people who would not necessarily be labeled "mathematical scientists." But the mathematical science content of such work, even if it is not research, is considerable, and therefore it is critical for the mathematical sciences community to play a role, through education, research, and collaboration. People with mathematical science backgrounds per se can bring different perspectives that complement those of computer scientists and others, and the combination of talents can be very powerful. The theoretical branches of many other fields—for instance, biology, ecology, engineering, economics—merge seamlessly with the mathematical sciences captures an important characteristic of the mathematical sciences—namely, that they overlap with many other disciplines of science, engineering, and medicine, and, increasingly, with areas of business such as finance and marketing. Where the small ellipses overlap with the main ellipse (representing the mathematical sciences), one should envision a mutual entwining and meshing, where fields overlap and where research and people might straddle two or more disciplines. Some people who are clearly affiliated with the mathematical sciences may have extensive interactions and deep familiarity with one or more of these overlapping disciplines.

And some people in those other disciplines may be completely comfortable in mathematical or statistical settings, as will be discussed further. These interfaces are not clean lines but instead are regions where the disciplines blend. A large and growing fraction of modern science and engineering is "mathematical" to a significant degree, and any dividing line separating the more central and the interfacial realms of the mathematical sciences is sure to be arbitrary. It is easy to point to work in theoretical physics or theoretical computer science that is indistinguishable from research done by mathematicians, and similar overlap occurs with theoretical ecology, mathematical biology, bioinformatics, and an increasing number of fields. This is not a new phenomenon—for example, people with doctorates in mathematics, such as Herbert Hauptman, John Pople, John Nash, and Walter Gilbert, have won Nobel prizes in chemistry or economics—but it is becoming more widespread as more fields become amenable to mathematical representations. This explosion of opportunities means that much of twenty-first century research is going to be built on a mathematical science foundation, and that foundation must continue to evolve and expand.

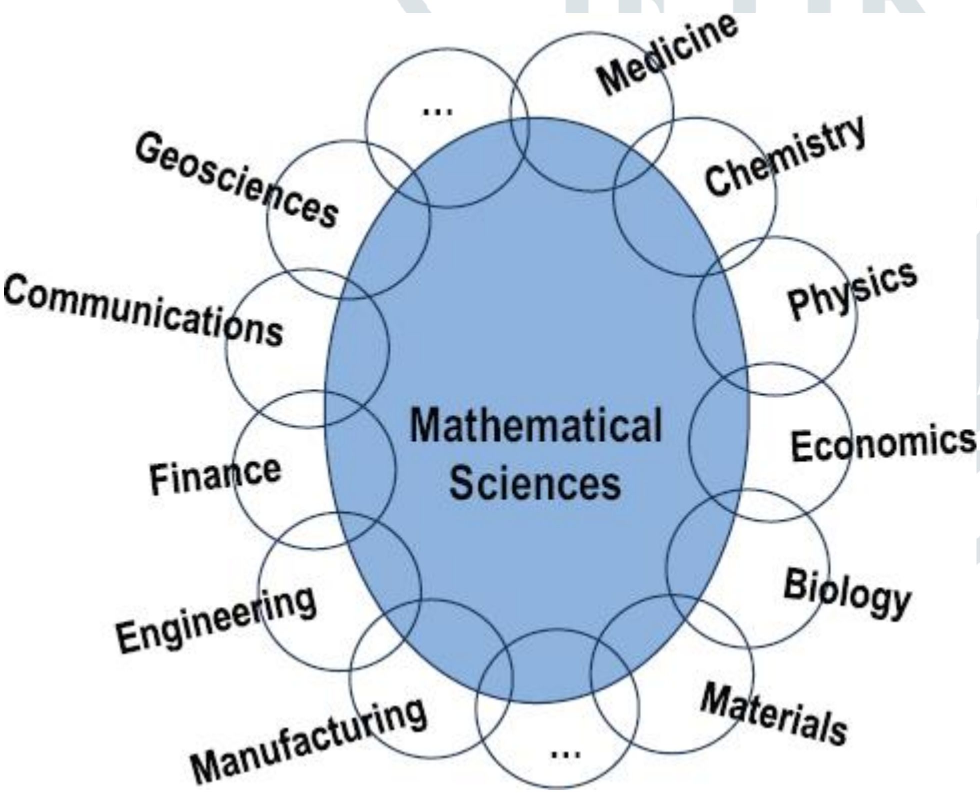
Objective:

This paper intends to explore and analyse the interrelationship between Physics, Mathematics and Chemistry, as time progressed, increasingly sophisticated mathematics started to be used in physics

BROADENING THE DEFINITION OF THE MATHEMATICAL SCIENCES

There is no precise definition of "the mathematical sciences." The following definition was used in the 1990 report commonly known as the David II report after the authoring committee's chair, Edward E. David:

The discipline known as the mathematical sciences encompasses core (or pure) and applied mathematics, plus statistics and operations research, and extends to highly mathematical areas of other fields such as theoretical computer science.



Distinctions between "core" and "applied" mathematics increasingly appear artificial; in particular, it is difficult today to find an area of mathematics that does not have relevance to applications. It is true that some mathematical scientists primarily prove theorems, while others primarily create and solve models, and professional reward systems need to take that into account. But any given individual might move between these modes of research, and many areas of specialization can and do include both kinds of work. Overall, the array of mathematical sciences share a commonality of experience and thought processes, and there is a long history of insights from one area becoming useful in another.

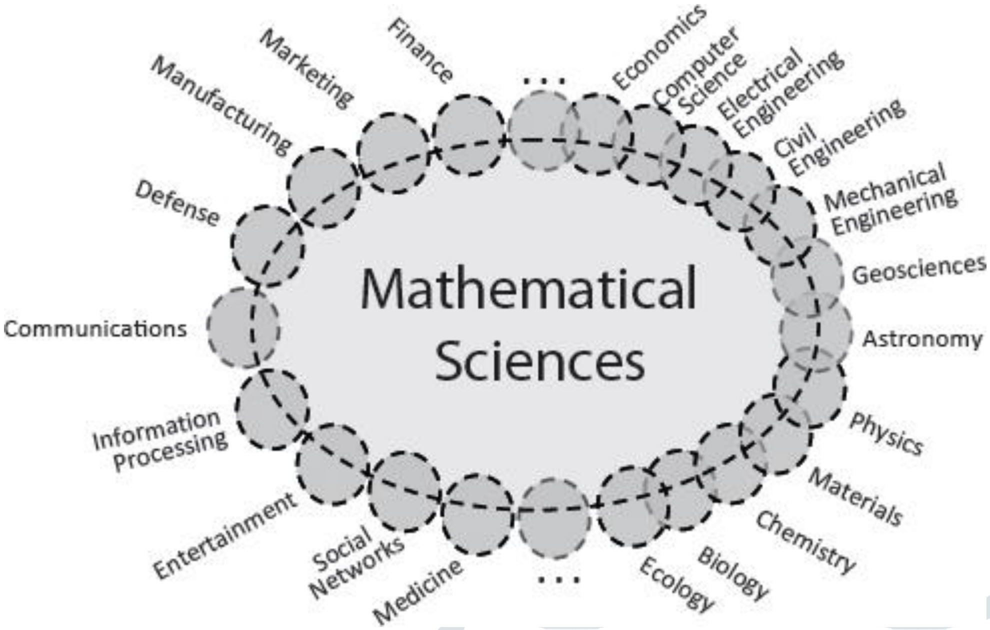
A long-standing practice has been to divide the mathematical sciences into categories that are, by implication, close to disjoint. Two of the most common distinctions are drawn between "pure" and "applied" mathematics, and between "mathematics" and "statistics." These and other categories can be useful to convey real differences in style, culture and methodology, but in the Panel's view, they have produced an increasingly negative effect when the mathematical sciences are considered in the overall context of science and engineering, by stressing divisions rather than unifying principles. Furthermore, such distinctions can create unnecessary barriers and tensions within the mathematical sciences community by absorbing energy that might be expended more productively. In fact, there are increasing overlaps and beneficial interactions between different areas of the mathematical sciences. . . . [T]he features that unite the mathematical sciences dominate those that divide them.[2]

Experience and all the sciences

What is this commonality of experience that is shared across the mathematical sciences? The mathematical sciences aim to understand the world by performing formal symbolic reasoning and computation on abstract structures. One aspect of the mathematical sciences involves unearthing and understanding deep relationships among these abstract structures. Another aspect involves capturing certain features of the world by abstract structures through the process of modeling, performing formal reasoning on these abstract structures or using them as a framework for computation, and then reconnecting back to make predictions about the world—often, this is an iterative process. A related aspect is to use abstract reasoning and structures to make inferences about the world from data. This is linked to the quest to find ways to turn empirical observations into a means to classify, order, and understand reality—the basic promise of science. Through the mathematical sciences, researchers can construct a body of knowledge whose interrelations are understood and where whatever understanding one needs can be found and used. The mathematical sciences also serve as a natural conduit through which concepts, tools, and best practices can migrate from field to field.

A further aspect of the mathematical sciences is to investigate how to make the process of reasoning and computation as efficient as possible and to also characterize their limits. It is crucial to understand that these different aspects of the mathematical sciences do not proceed in isolation from one another. On the contrary, each aspect of the effort enriches the others with new problems, new tools, new insights, and—ultimately—new paradigms.

The traditional areas of the mathematical sciences are certainly included. But many other areas of science and engineering are deeply concerned with building and evaluating mathematical models, exploring them computationally, and analyzing enormous amounts of observed and computed data. These activities are all inherently mathematical in nature, and there is no clear line to separate research efforts into those that are part of the mathematical sciences and those that are part of computer science or the discipline for which the modeling and analysis are performed.[3] The committee believes the health and vitality of the discipline are maximized if knowledge and people are able to flow easily throughout that large set of endeavors.



So what is the "mathematical sciences community"? It is the collection of people who are advancing the mathematical sciences discipline. Some members of this community may be aligned professionally with two or more disciplines, one of which is the mathematical sciences. (This alignment is reflected, for example, in which conferences they attend, which journals they publish in, which academic degrees they hold, and which academic departments they belong to.) There is great value in the mathematical sciences welcoming these "dual citizens"; their involvement is good for the mathematical sciences, and it enriches the ways in which other fields can approach their work.

Science bioinformatics, and other areas

The collection of people in the areas of overlap is large. It includes statisticians who work in the geosciences, social sciences, bioinformatics, and other areas that, for historical reasons, became specialized offshoots of statistics. It includes some fraction of researchers in scientific computing and computational science and engineering. It includes number theorists who contribute to cryptography, and real analysts and statisticians who contribute to machine learning. It includes operations researchers, some computer scientists, and physicists, chemists, ecologists, biologists, and economists who rely on sophisticated mathematical science approaches. Some of the engineers who advance mathematical models and computational simulation are also included. It is clear that the mathematical sciences now extend far beyond the definitions implied by the institutions—academic departments, funding sources, professional societies, and principal journals—that support the heart of the field.

As just one illustration of the role that researchers in other fields play in the mathematical sciences, the committee examined public data[4] on National Science Foundation (NSF) grants to get a sense of how much of the research supported by units other than the NSF Division of Mathematical

Sciences (DMS) has resulted in publications that appeared in journals readily recognized as mathematical science ones or that have a title strongly suggesting mathematical or statistical content. While this exercise was necessarily subjective and far from exhaustive, it gave an indication that NSF's support for the mathematical sciences is de facto broader than what is supported by DMS. It also lent credence to the argument that the mathematical sciences research enterprise extends beyond the set of individuals who would traditionally be called mathematical scientists. This exercise revealed the following information:

• Grants awarded over the period 2008-2011 by NSF's Division of Computing and Communication Foundations (part of the Directorate for Computer and Information Science and Engineering) led to 262 publications in the areas of graphs and, to a lesser extent, foundations of algorithms.

• Grants awarded over 2004-2011 by the Division of Physics led to 148 publications in the general area of theoretical physics.

• Grants awarded over 2007-2011 by the Division of Civil, Mechanical, and Manufacturing Innovation in NSF's Engineering Directorate led to 107 publications in operations research.

This cursory examination also counted 15 mathematical science publications resulting from 2009-2010 grants from NSF's Directorate for Biological Sciences. (These publication counts span different ranges of years because the number of publications with apparent mathematical sciences content varies over time, probably due to limited-duration funding initiatives.) For comparison, DMS grants that were active in 2010 led to 1,739 publications. Therefore, while DMS is clearly the dominant NSF supporter of mathematical science research, other divisions contribute in a nontrivial way.

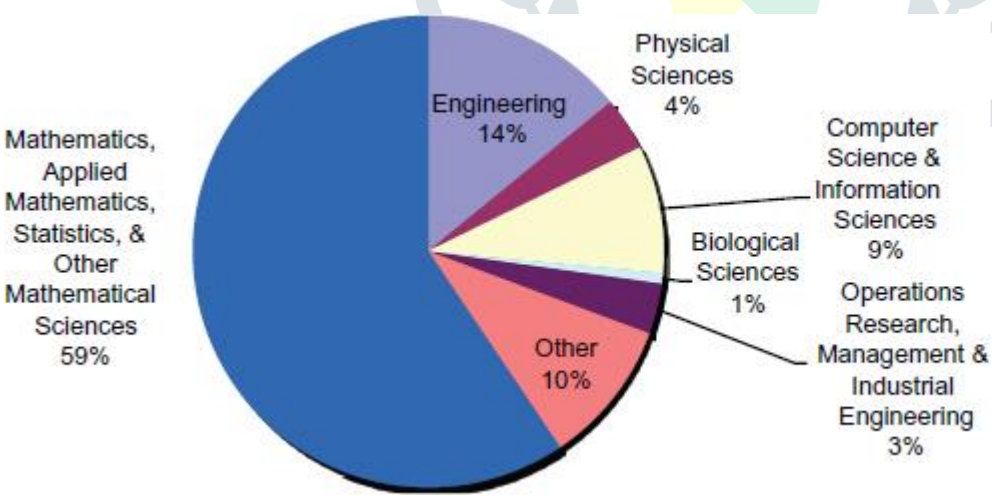
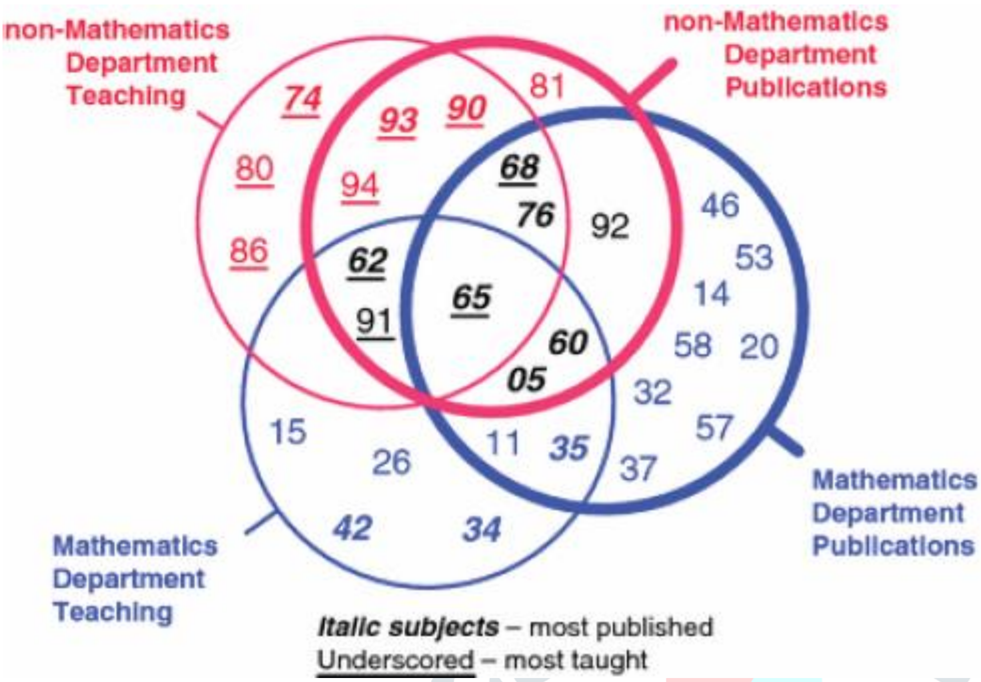


FIGURE 3-3 SIAM members identify the primary department with which they are affiliated. This figure shows the fraction of 6,269 nonstudent members identifying with a particular category.

IMPLICATIONS OF THE BROADENING OF THE MATHEMATICAL SCIENCES

The tremendous growth in the ways in which the mathematical sciences are being used stretches the mathematical science enterprise—its people, teaching, and research breadth. If our overall research enterprise is operating well, the researchers who traditionally call themselves mathematical scientists—



TWO MAJOR DRIVERS OF EXPANSION: COMPUTATION AND BIG DATA

Two factors have combined to spark the enormous expansion of the role of the mathematical sciences: (1) the widespread availability of computing power and the consequent reliance on simulation via mathematical models by so much of today's science, engineering, and technology and (2) the explosion in the amount of data being collected or generated, which often is of a scale that it can only be evaluated through mathematical and statistical techniques.

As science, engineering, government, and business rely increasingly on complex computational simulations, it is inevitable that connections between those sectors and the mathematical sciences are strengthened. That is because computational modeling is inherently mathematical. Accordingly, those fields depend on—and profit from—advances in the mathematical sciences and the maintainance of a healthy mathematical science enterprise. The same is true to the extent that those sectors increasingly rely on the analysis of large-scale quantities of data.

This is not to say that a mathematical scientist is needed whenever someone builds or exercises a computer simulation or analyzes data (although the involvement of a mathematical scientist is often beneficial when the work is novel or complex). But it is true that more and more scientists, engineers, and business people require or benefit from higher-level course work in the mathematical sciences, which strengthens connections between disciplines. And it is also true that the complexity of phenomena that can now be simulated in silico, and the complexity of analyses made possible by terascale data, are pushing research frontiers in the mathematical sciences and challenging those who could have previously learned the necessary skills as they carry out their primary tasks. As this complexity increases, we are finding more and more occasions where specialized mathematical and statistical experience is required or would be beneficial.

Some readers may assume that many of the topics mentioned in this chapter fall in the domain of computer science rather than the mathematical sciences. In fact, many of these areas of inquiry straddle both fields or could be labeled either way. For example, the process of searching data, whether in a database or on the Internet, requires both the products of computer science research and modeling and analysis tools from the mathematical sciences. The challenges of theoretical computer science itself are in fact quite mathematical, and the fields of scientific computing and machine learning sit squarely at the interface of the mathematical sciences and computer science (with insight from the domain of application, in many cases). Indeed, most modeling, simulation, and analysis is built on the output of both disciplines, and researchers with very similar backgrounds can be found in academic departments of mathematics, statistics, or computer science. There is, of course, a great deal of mathematical sciences research that has not that much in common with computer sciences research—and, likewise, a great deal of computer science research that is not particularly close to the mathematical sciences.

Collaboration and breakthroughs

The reason is that mathematical science researchers not only create the tools that are translated into applications elsewhere, but they are also the creative partners who can adapt mathematical sciences results appropriately for different problems. This latter sort of collaboration can result in breakthrough capabilities well worth the investment of time that is sometimes associated with establishing a cross-disciplinary team. It is not always enough to rely on the mathematics and statistics that is captured in textbooks or software, for two reasons: (1) progress is continually being made, and off-the-shelf techniques are unlikely to be cutting edge, and (2) solutions tailored to particular situations or questions can often be much more effective than more generic approaches. These are the benefits to the nonmathematical sciences members of the team. For mathematical science collaborators, the benefits are likewise dual: (1) fresh challenges are uncovered that may stimulate new results of intrinsic importance to the mathematical sciences and (2) their mathematical science techniques and insights can have wider impact.

In application areas with well-established mathematical models for phenomena of interest—such as physics and engineering—researchers are able to use the great advances in computing and data collection of recent decades to investigate more complex phenomena and undertake more precise analyses. Conversely, where mathematical models are lacking, the growth in computing power and data now allow for computational simulations using alternative models and for empirically generated relationships as means of investigation.

Computational simulation now guides researchers in deciding which experiments to perform, how to interpret experimental results, which prototypes to build, which medical treatments might work, and so on. Indeed, the ability to simulate a phenomenon is often regarded as a test of our ability to understand it. Over the past 10-15 years, computational capabilities reached a threshold at which statistical methods such as Markov chain Monte Carlo methods and large-scale data mining and analysis became feasible, and these methods have proved to be of great value in a wide range of situations.

For example, at one of its meetings the study committee saw a simulation of biochemical activity developed by Terrence Sejnowski of the Salk Institute for Biological Studies. It was a tour de force of computational simulation—based on cutting-edge mathematical sciences and computer science—that would not have been feasible until recently and that enables novel investigations into complex biological phenomena. As another example, over the past 30 years or so, ultrasound has progressed from providing still images to dynamically showing a beating heart and, more recently, to showing the evolution of a full baby in the womb. The mathematical basis for ultrasound requires solving inverse problems and draws

CONTRIBUTIONS OF MATHEMATICAL SCIENCES TO INDUSTRY

The role of the mathematical sciences in industry has a long history, going back to the days when the Egyptians used the 3-4-5 right triangle to restore boundaries of farms after the annual flooding of the Nile. That said, the recent period is one of remarkable growth and diversification. Even in old-line industries, the role of the mathematical sciences has expanded. For example, whereas the aviation industry has long used mathematics in the design of airplane wings and statistics in ensuring quality control in production, now the mathematical sciences are also crucial to GPS and navigation systems, to simulating the structural soundness of a design, and to optimizing the flow of production. Instead of being used just to streamline cars and model traffic flows, the mathematical sciences are also involved in the latest developments, such as design of automated vehicle detection and avoidance systems that may one day lead to automated driving. Whereas statistics has long been a key element of medical trials, now the mathematical sciences are involved in drug design and in modeling new ways for drugs to be delivered to tumors, and they will be essential in making inferences in circumstances that do not allow double-blind, randomized clinical trials. The financial sector, which once relied on statistics to design portfolios that minimized risk for a given level of return, now makes use of statistics, machine learning, stochastic modeling, optimization, and the new science of networks in pricing and designing securities and in assessing risk.

What is most striking, however, is the number of new industries that the mathematical sciences are a part of, often as a key enabler. The encryption industry makes use of number theory to make Internet commerce possible. The “search” industry relies on ideas from the mathematical sciences to make the Internet’s vast resources of information searchable. The social networking industry makes use of graph theory and machine learning. The animation and computer game industry makes use of techniques as diverse as differential geometry and partial differential equations. The biotech industry heavily uses the mathematical sciences in modeling the action of drugs, searching genomes for genes relevant to human disease or relevant to bioengineered organisms, and discovering new drugs and understanding how they might act. The imaging industry uses ideas from differential geometry and signal processing to procure minimally invasive medical and industrial images and, within medicine, adds methods from inverse problems to design targeted radiation therapies and is moving to incorporate the new field of computational anatomy to enable remote surgery. The online advertising industry uses ideas from game theory and discrete mathematics to price and bid on online ads and methods from statistics and machine learning to decide how to target those ads. The marketing industry now employs sophisticated statistical and machine learning techniques to target customers and to choose locations for new stores. The credit card industry uses a variety of methods to detect fraud and denial-of-service attacks. Political campaigns now make use of complex models of the electorate, and election-night predictions rely on integrating these models with exit polls. The semiconductor industry uses optimization to design computer chips and in simulating the manufacture and behavior of designer materials. The mathematical sciences are now present in almost every industry, and the range of mathematical sciences being used would have been unimaginable a generation ago.

Conclusion

A prime example of how expanding computational and data resources have led to the “mathematization” of a field of science is the way that biology became much more quantitative and dependent on mathematical and statistical modeling following the emergence of genomics. High-throughput data in biology has been an important driver for new statistical research over the past 10-15 years.

Research in genomics and proteomics relies heavily on the mathematical sciences, often in challenging ways, and of disease, evolution, agriculture, and other topics have consequently become quantitative as genomic and proteomic information is incorporated as a foundation for research. Arguably, this development has placed statisticians as central players in one of the hottest fields of science. Over the next 10-15 years, acquiring genomic data will become fairly straightforward, and increasingly it will be available to illuminate biological processes.

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