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The state of multivariate thinking for scientists in industry: 1980–2000

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Abstract

Chemometrics has enjoyed tremendous success in the areas related to calibration of spectrometers and spectroscopy-based measurements. These chemometric-based spectrometers have been widely applied for process monitoring and quality assurance. However, chemometrics has the potential to revolutionize the very intellectual roots of problem solving. Are there barriers to a more rapid proliferation of chemometric-based thinking, particularly in industry? What are the potential effects of chemometrics technology and the New Network Economy (NNE) working in concert? Who will be the winners in the race for faster, better, cheaper systems and products? These questions are reviewed in terms of the principles of the NNE and in the promise of chemometrics for industry. What then is the state of multivariate thinking in industry? Several powerful principles are derived from an evaluation of the NNE and chemometrics which could allow chemometrics to proliferate much more rapidly as a key general problem-solving tool.

Keywords: Multivariate thinking; Spectrometer calibration; Spectroscopy-based measurements

1. Introduction

> In chemistry, one's ideas, however, beautiful, logical, elegant, imaginative… are simply without value unless they are actually applicable to the one physical environment we have; in short, they are only good if they work (R.B. Woodward).

1.1. Relating the theme of chemometrics to a busy technical community

Twenty years after the term chemometrics was freshly "minted," by Bruce Kowalski and Svante Wold, the chemometrics community still seems to be searching for a universal definition and a clear identity. This paper begins by examining several definitions for chemometrics, the clarity of these definitions and the message communicated to the industrial community.

> Chemometrics is what chemometricians do. Anon.

> Chemometrics has been defined as the application of mathematical and statistical methods to chemical measurements [1].

> Chemometrics is the chemical discipline that uses mathematical and statistical methods for the obtention in the optimal way of relevant information on material systems [2].

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> Chemometrics developments and the accompanying realization of these developments as computer software provide the means to convert raw data into information, information into knowledge and finally knowledge into intelligence [3].

> Analytical chemistry has been called a science without a theory. Some say that the theories and principles of analytical chemistry have been handed down from other branches of science. Developments in chemometrics that are beginning to effect instrument design and specify the limits of analysis are shaping the foundation for this science…research in chemometrics will contribute to the design of new types of instruments, generate optimal experiments that yield maximum information, and catalog and solve calibration and signal resolution problems. All this while quantitatively specifying the limitations of each instrument as well as the quality of the data it generates [4].

> Chemometrics, the application of statistical and mathematical methods to chemistry…[5].

> Chemometrics is the discipline concerned with the application of statistics and mathematical methods, as well as those methods based on mathematical logic, to chemistry [6].

> Chemometrics is the discipline concerned with the application of statistical and mathematical methods, as well as those methods based on mathematical logic, to chemistry [7–9].

> Chemometrics can generally be described as the application of mathematical and statistical methods to (1) improve chemical measurement processes and (2) extract more useful information from chemical and physical measurement data [10].

> Chemometrics is an approach to analytical and measurement science based on the idea of indirect observation. Measurements related to the chemical composition of a substance are taken, and the value of a property of interest is inferred from them through some mathematical relation [11].

> Chemometrics (this is an international definition) is the chemical discipline that uses mathematical and statistical methods, (a) to design or select optimal measurement procedures and experiments; and (b) to provide maximum chemical information by analyzing chemical data [12].

From these definitions, we are left with a few nearly irrefutable facts: chemometrics involves chemistry and math….most probably data, and possibly sensors and measurements of processes. Whatever the clear and present definition of chemometrics is, the industrial understanding of it is that it is complicated, it requires computers and that it could possibly be beneficial. However, we are not exactly certain how or why it would be an advantage to use chemometrics. The fact is that chemometrics allows us to take off the shelf data, which many institutions have been generating ad infinitum, and "wring it out" to remove all the information content. This information can further be scrutinized to obtain real knowledge of processes and measurements: knowledge for optimized and new products, processes, intellectual property estates, at reduced cost.

Chemometrics is so often linked with Process Analytical Chemistry, again defined by Kowalski "as the discovery and development of new and sophisticated analytical methods for use in-line as an integral part of automated chemical processes [13]." Some have said that process analytical chemistry is 90% hardware and 10% chemometrics. To an engineer that quantitative statement means one may be able to do without it. What we have then is a process—we make measurements—we collect data—we use chemometrics to obtain information—we review the information and attain real knowledge. If chemometrics is difficult to clearly define and communicate, what are its advantages and disadvantages?

2. Advantages of chemometrics

What then are the clear advantages of chemometrics?

1. Chemometrics provides speed in obtaining real-time information from data.

2. It allows high quality information to be extracted from less resolved data.
3. It provides clear information resolution and discrimination power when applied to second, third and possibly higher-order data.
4. It provides methodology for cloning sensors—for making one sensor take data “precisely“ as another sensor.
5. It provides diagnostics for the integrity and probability that the information it derives is accurate.
6. It promises to improve measurements.
7. It improves knowledge of existing processes.
8. It has very low capital requirements—it’s cheap.

In summary, it provides the promise of faster, cheaper, better information with known integrity. In addition, it is common sense to know that math is cheaper than physics—that computer programs that can solve problems that traditionally have required extensive hardware developments and advances; it represents a superior approach. We see then that intelligence can replace physical and material solutions as much as the digital chip replaces the mechanical clock works. This is an important theme to further develop.

2.1. Case study: a successful application of chemometrics has been in spectroscopic analysis

Recent reviews describing the remarkable proliferation of near-infrared, infrared and Raman chemometrics-based analyzers for use in process analysis are given in references [14–21]. These references and many others cite several thousand cases where chemometrics was applied to calibration of sensors to analyze complex chemical mixtures and used for on-line or at-line analysis. Without chemometrics most, if not all, of these applications would not have been possible. What made these particular applications of chemometrics, in the broadest sense, work. In fact, multivariate calibration is commonly accepted for process, research and quality use applications throughout the world of spectroscopy.

Chemometric-based spectrometers provide rapid information enabling real-time process change capabilities and the advanced diagnosis of potential process upsets. Many companies have already recognized the value-added nature of these process analytical technologies. The main benefits for process spectroscopy include: (1) safer plant and process operations through real-time monitoring and prevention of potentially dangerous process upsets; (2) assurance that processes and plant environments are in compliance to environmental regulations; (3) an increase in process plant operability through timely adjustments in processes possible using real-time data; (4) improved product quality through maintenance of tighter control limits; (5) minimization of waste products through process optimization; (6) product production cost minimization through tighter target limits and more accurate production scheduling; (7) optimization of production capacity resulting from increased process operability and continuous product quality verification [11]. In addition, rapid screening for product verification analysis yields improved safety and quality control for pharmaceutical companies. The economic value of achieving these results is high, yet the cost of implementation is relatively low. In the future, accurate and reliable multicomponent sensors for complex processes or tiny monitors for specific analytes will undoubtedly be common. Microtooling and advances in sensor and microprocessor technologies may indeed produce future reductions in the size and cost of process sensors.

What can be learned about these successes, and where is the state of spectroscopic analysis using chemometrics in industry today? The field of process analytical chemistry using chemometrics is expanding due to the economic and regulatory benefits achieved by using rapid and accurate information. This simple concept allows process optimization with resultant improved productivity, efficiency and product quality; with the additional benefit of reduced waste products. Near-infrared, infrared, and Raman spectroscopy fit well into the list of technologies suitable for process analysis involving chemometrics; they are fast, precise and nondestructive analytical techniques. When used properly they are also accurate for macroanalysis of major chemical components and contaminants in process and manufacturing situations. These measurements use quantitative and qualitative chemometric techniques, which are receiving more widespread acceptance within the analytical community.

3. Disadvantages of chemometrics

The perceived disadvantage of chemometrics is that there is widespread ignorance about what it is and what it can realistically accomplish. The notion that 'many people talk about chemometrics, but there are relatively few actually using it for daily activities and major problem solving in industrial situations.' This science is considered too complex for the average technician and analyst. The mathematics can be misinterpreted as esoteric and not relevant. Most importantly, for the industry, there are a dismal lack of official practices and methods associated with chemometrics.

Chemometrics requires a change in one's approach to problem solving from univariate to multivariate thinking since we live in an essentially multivariate context. From pondering over spreadsheets to actually analyzing the data for its full information content. The old scientific method is passing away; a new scientific method is arising from its ashes. A new method requiring not a thought ritual but rather a method involving many inexpensive measurements, possibly a few simulations and chemometric analysis. The new method looks at all the data from a multivariate approach, whereas the old method requires the scientist's assumed powers of observation from a univariate standpoint to be the key data processor.

The old scientific method (used for hundreds of years) are as follows:

1. Stating the problem;
2. Forming the hypothesis;
3. Observing and experimenting;
4. Interpreting data (traditionally univariate—pondering stage);
5. Drawing conclusions.

The new scientific method (for problem solving) are as follows:

1. Measure a process (any chemical phenomenon or process);
2. Analyze the data (multivariate analysis);
3. Iterate if necessary;
4. Create and test model;
5. Develop fundamental multivariate understanding of the process.

4. Examples of reluctance to change

Industry relies on approved and accepted methods which can easily be defended in a court of law. The implementation of methods must involve a minimum of risk to the user and to the organization sponsoring the user. Historically, most NIR papers use Ordinary Least Squares to compare predicted NIR results against laboratory results. However, some regulatory groups have questioned the use of least squares and associated multivariate calibration for analytical methods involved with product release or compliance.

An Official ASTM document, "Standard Practices for Infrared, Multivariate, Quantitative Analyses," has recently been published [22]. This 25-page document is designated E1655-97 and includes "a guide for the multivariate calibration of infrared spectrometers used in determining the physical or chemical characteristics of materials." The practice applies to "the Near-Infrared (NIR) spectral region (roughly 780 to 2500 nm) through the Mid Infrared (MIR) spectral region (roughly 4000 to 400 cm^{-1})." In addition, the Practice also includes: procedures for collecting and treating data for developing IR calibrations; definitions for terms and calibration techniques; and criteria for validating the performance of a calibration model.

Other "official" analytical methods exist utilizing *multivariate* chemometric practices for calibration. The methods briefly described below are the major documents in existence. In all cases, the approval procedure for these methods or practices involved multiple peer reviews and technical working groups operating on a voluntary basis for a period of years. The second method is published by the Association of Official Analytical Chemists (AOAC) as Method 989.03, 1989 [23]. This publication presents a near-infrared method for the determination of Acid Detergent Fiber and Crude Protein in forage materials using multivariate calibration. This method is also referenced in the JAOAC, 71, 1162 (1988). The method describes sample preparation and calibration procedures. The third method published is from the American Association of Cereal Chemists (AACC) Method 39-10 [24] describing a near-infrared method for protein determination in all classes of wheat based on near-infrared reflectance spectroscopy. This is a general method for protein calibration based on data from filter or full wavelength near-infrared instruments. The specifics related to calculating the calibration coefficients are not given.

Why then is the use of chemometrics for *official* analytical methods is still in its early stages? Part of the reason for this is the need for chemometricians to be involved in drafting (or codifying) best practices and official methods for using chemometrics. Since many of the calibration techniques are nonautomated, they naturally required expert manual labor to *provide the hands-on automation*. There is still a great deal of art involved in the various approaches to calibration. In order to convince the industrial community of its usefulness, chemometric practices should be codified by peer-reviewed scientific organizations and placed into practices and software code for implementation. This can only be accomplished using highly skilled chemometricians and application scientists meeting in concert to perform these tasks. With such developments, the technology could move forward more rapidly than is currently possible. Barriers to more rapid proliferation of chemometric-based techniques include:

1. It is still considered new technology;
2. Few "official" methods and practices are available;
3. It is considered technically complex and nonintuitive (esoteric and requiring a specialist); and
4. It cannot be automated until it is scientifically codified.

5. Case study: lessons for chemometrics from the New Network Economy (NNE)

5.1. Rules of the NNE [25]

To start, let us look at two provocative statements relating to the new economy: "Give it away and it becomes priceless...keep it for yourself and it becomes worthless, " and "One fax machine is worthless, two are extremely valuable, many are priceless...." In the new economy increased complexity is the friend of confusion and chaos. The average person remembers 7 ± 2 objects per human byte and the modes of communication provide multichannel competition for any concept. Among other means of communication, there is mobile connection commerce, Internet commerce, direct print, television, radio, telephone and fax commerce and direct human contact. Concepts must then be clearly formulated and communicated to have any meaningful impact.

To be fast and first requires risk taking, risk by definition has a high failure rate. The lesson is to expend energy reducing the cost of risk, not the rate of risk. One must make it more expensive to be slow than wrong. So what are the laws of the NNE? This theme is expanded in a later discussion.

1. The world is moving toward connectedness.
2. Services become more valuable the more plentiful they are.
3. Networked systems grow exponentially.
4. Success becomes infectious.
5. Value explodes with membership.
6. Cost goes down the better and more valuable the services are.
7. The more of something given free, the more valuable it becomes—wealth feeds off ubiquity.
8. Allegiances move away from organizations and toward networks.
9. Devolution is essential—grassroots and bottoms-up (users) are in control.
10. A move from atoms to bits—smaller, smarter electronic systems over mechanical solutions.
11. Sustainable disequilibrium—constant change is the order of things.
12. Find the right task, not how to do the wrong task better.

The "new network economy" is not mostly about personal web pages and fanciful graphics—it's about new technology changing costs and communications possibilities. Prior to the printing press, a single book would cost US$400,000.00. 100 years after the telephone was introduced as two terminals, there were 643 billions calls per year made in America alone (1997 statistics). Massive changes in underlying costs create massive new opportunities. Assumption to knowledge ratio causes more problems than ever before:

1. In the new economy, experience can be your worst enemy—it can lie to you about today's reality.
2. Technologies must maximize learning rate while minimizing cost.
3. Technological approaches must reduce the cost of failure, not the rate of failure.

In summary, you can fail often if you fail cheaply.

5.2. The human attention resource limitation

In the new economy there is a shift in the resource equation.

Resource equation

Scarce	Plentiful
Time	Money
Talent	Computing power
Attention	Network services
Motivation for change	Confidence in status quo
Risk-taking incentive	Let Mikey try it—if he fails, we will "demote" him

If *human attention* is one of the key resource problems in the NNE, then clear communications is key. Unfortunately, in an ever increasing age of specialization, we find ourselves suffering from the stovepipe effect. This effect has each individual group of specialists separated by function and by technical language. This causes a stovepipe organization where R&D scientists, R&D engineers, Product managers, Quality Assurance, Manufacturing, Financial, Administrative, Logistical and others really do not communicate well; thus, horizontal communication fails. Tools to break down this effect include clear symbolic communication and incentives directed toward the correct behaviors. People like to be recognized for contributions. Clear, objective, visible, awards calibrated to the actual achievement or contribution are valuable for motivating technical workers.

Let us examine these principles as they apply to any obstacles to implementation of chemometrics. The process decisions are in the domain of the chemical engineer, plant manager and quality group. Their process decisions are based upon process modeling, temperature, pressure, flow and mass balance, which are considered adequate and always have been adequate. Decisions are made in the plant and through various engineering groups. These decisions are made based upon past experience and current academic training. The reason then that changes are so slow, and most resist change to include chemometric-based sensors is precisely due to resource deficiencies—in time, talent, attention, motivation and risk-taking incentive.

The process engineer and manufacturing personnel require motivators to change behavior patterns, such as: recognition for accomplishment, demonstrated process improvement, no risk, convenience, economical choices; thus, the risk/reward ratio must be near zero. The company has a separate list of requirements, such as: improved process performance, increased profits, maintenance or improvements in quality, convenience, economical to implement, low risk; thus, the [Rewards/(Risk + Cost)] ratio must be a very large number.

Chemometrics supplies a perfect fit to these requirements by providing the expertise (time and talent) into the resource equation, by minimizing cost by data-analysis techniques requiring some sensor and computer time, and demonstrating a potential benefit in understanding a process providing priceless information for improving it.

5.3. When should chemometrics be applied in industry?

In the relentless pursuit of technical truth and cooperation, the chemometrician will be subjected to many trials including several questions. These will inevitably include those such as, why is chemometrics better than the math I learned in engineering school? Don't all the sensor vendors know this math—in fact, don't they mostly have proprietary algorithms? Can we sell more of our product if we put these chemometric sensors on line? The project or team leader must quiz their own internal customer. The questions asked will include multiple technical details, but also questions related to where one could best apply chemometrics, what are the subgroups within that working space (personnel and projects), what circumstances prompt the use of chemometrics, what are the expected outcomes and how will these be implemented when completed.

It is important from a company standpoint to differentiate chemometric approaches for different applications using some recommended tools. To evaluate a project from a project engineering viewpoint is useful. Mapping the problem using tools similar to Tables 1–3 is a useful exercise to keep a project team on track. Using checklists to review progress is also extremely valuable.

Check list for making chemometric sensors work:

- Test underlying assumptions continually and thoroughly at lowest possible cost.
- Prepare multiple alternatives solutions.
- Commit to technology, but not to one use or application of technology—look for multiple uses.
- Control time and cost commitment issues.
- Avoid overload of staff-2 substantial projects each is the optimum number.
- Are there an internal customer market for this technology or approach?
- Can we deliver the technology reliably and cost effectively?
- Can we take small exploratory forays into less challenging opportunities, learning and adapting as we proceed?
- Continually codify and diffuse the information relative to project, including risks, potential benefits, and proposed solutions.

5.4. *The new rules of value in technology [26,27]*

There is a new energy revolution about this. In this new revolution, the rules are changing rapidly. For example, in the Neolithic Age, renewable energy sources were used to produce food (i.e., spear has high energy content and low information content). In the Industrial Age, nonrenewable energy sources were used to produce goods (i.e., mechanical devise has lower human energy input than spear with much higher information content). In the Information Age, information is substituted for energy to produce knowledge-intensive goods (i.e., the Pentium chip requires less energy than mechanical devise, but has much greater information content).

Table 2
Chemometrics project portfolio (potential cost vs. risk score = 1–9)

Relative cost of project			
High (3)	3	6	9
Medium (2)	2	4	6
Low (1)	1	2	3
Technical risk (uncertainty of sensor(s) and chemometrics used in approach)	Low (1)	Medium (2)	High (3)

The paradox of value occurs in the NNE. In the old economy, value was equal to the sum of utility and scarcity. In the NNE model, value is equal to the sum of utility and ubiquity. “First, wealth in this new regime flows directly from innovation, not optimization; that is, wealth is not gained by perfecting the known, but by imperfectly seizing the unknown. Second, the ideal environment for cultivating the unknown is to nurture the supreme agility and nimbleness of networks, Third, the domestication of the unknown inevitably means abandoning the highly successful known—undoing the perfected. And last, in the thickening web of the Network Economy, the cycle of ‘find, nurture, destroy’ happens faster and more intensely than ever before [27].”

Table 1
Industrial chemometrics attribute map—assists in answering the question as to when to extend the traditional use of measurement techniques using advances in multivariate analysis and computational approaches. For example, is regulatory compliance and reliability the Basic requirements of the analysis method or is real-time data? What performance attributes make using computational approaches attractive, and which attributes may suggest the use of these techniques may be inadvisable?

	Basic	Discriminator	Energizers
Attribute no.	Non-negotiable (Must have)	Differentiator (Yields an improvement over a basic solution)	Exciter (Is truly a motivator providing potentially outstanding results)

Table 3
Chemometrics project portfolio (project selection score = 1–27)

Cost vs. risk score			
High (6+)	18–27	12–18	6–9
Medium (3+)	9–15	6–10	3–5
Low (1+)	3–6	2–4	1–2
Value to corporation (US$)	Low (3)	Medium (2)	High (1)

Select lowest score projects first and don't often venture above 6.

5.5. *Who will take the lead in chemometrics or other technology?*

Why don't the large firms take an interest—with all their technology? The big firms won't accept low gross margins—or "smaller" opportunities (i.e., markets). The disruptive technologies are initially financially unattractive to incumbents, but not new entrants. Several known properties or characteristics exist relative to new technologies like chemometrics. The properties of innovative change in technology include:

1. New technologies are usually inferior to present state of the art.
2. Today's technology leaders dismiss the new technology.
3. New technology moves forward very rapidly only after take-off.
4. Success creates the seeds of its own failure due to arrogance.
5. Competency traps itself in the status quo.
6. To survive, the competent must seek to replace themselves with new competencies. Old technology insists on improved execution of the wrong thing, not an emphasis on doing the right thing.

As humans, we learn best by discussion, active participation and by teaching others, very few learn or retain much by lecture or reading complex material. There is inertia against changing and inertia produced once something is learned or established. Changing from the old to the new requires commitment, leadership and a clear message. Change is difficult—and always has been. "There is nothing more difficult to plan, more doubtful of success or more dangerous to manage than the creation of a new system. For the initiator has the enmity of all who would profit by the preservation of the old institutions and merely lukewarm defenders in those who would gain by the new ones. The hesitation of the latter arises in the part from their fear of their adversaries, who have the laws on their side, and in part from the general skepticism of mankind which does not really believe in an innovation until experience proves its value. So it happens that whenever his enemies have occasion to attack the innovator, they do so with the passion of partisans, while the others defend him sluggishly, so that the innovator and party alike are vulnerable [28]."

Those in current power (for lack of a better term) will inevitably proceed through several steps when confronted with undeniable facts about the advantages of a new system or technology. These include, in order of occurrence: (1) denial, (2) resistance, (3) negotiation, and (4) acceptance. In order to move people through the stages of acceptance of change and even to the act of embracing the changes must involve: (1) empathy—realization that change is a most difficult human activity, (2) information sharing—keeping everyone informed as much as possible, and (3) involvement—involving the group as a team.

There is a new model for failure in the NNE. Managing adaptation and change in a counter intuitive new world is difficult. However, in the NNE, failure is expected and managed. One must fail fast, fail cheap, and move on. One must regard failure a means of learning what will be successful. One could say that the size of your scrap heap indicates the learning potential for future success [29].

6. Is calibration all chemometrics has to offer?

Calibration of infrared and near-infrared spectrometers has been far and away the most noted use of chemometrics in industry. However, is this the best and most desirable use of this powerful technology? Do industrial managers get excited about calibrating a sensor using a new optimized technique, or in answering the question as to whether PLS is better than PCR in this or that case? I think not. In fact, the sensors are all supposed to make some measurement using all those optics and electronics in the box—and that is that! Most chemometric books discuss mostly the aspects of calibration with a few miscellaneous applications. Examples [30,31] are adequate to demonstrate this principle.

Nowadays, industry may be missing something, and with all deference to the authors of these texts; however, this material is still uncodified (esoteric) and undiffused (not distributed for general consumption) and it looks like through chemometrics, one mostly has tools for calibration—some for quantitative analysis, some for qualitative—analysis techniques using the various forms of multivariate analysis and pattern recognition techniques. What else is there? How about codifying the concept of applying the principles of multivariate thinking to every possible problem that suffers from "univariatism."

7. Examples of high appeal chemometric projects

7.1. Example 1

Twenty-eight tedious manual tests are routinely performed on properties of product A′ manufactured using process A. Some unknown variation causes marked improvement in product A′ (resulting in a new invention), see Figs. 1 and 2. Univariate analysis of test data shows nothing, yielding an unexplainable change in the product A′. Multivariate analysis using PCA and interpretation of eigenvectors shows that four specific properties are important to produce the improved product A′.

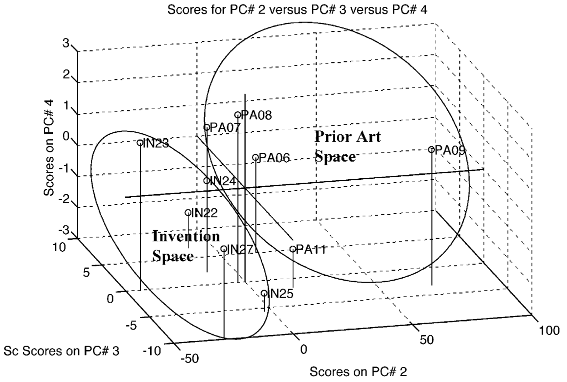

Fig. 1. Scores plot of PC2, PC3, and PC4 for product A′ (Invention Space) samples vs. old product A (Prior Art Space) samples as discriminated using PCA on mean centered data.

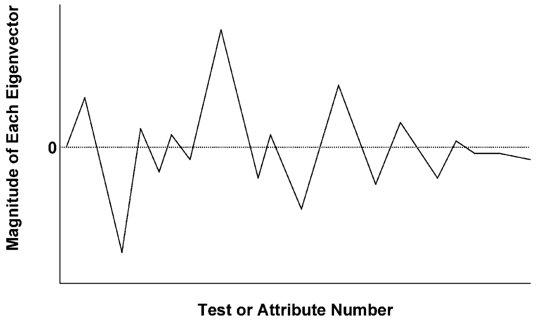

Fig. 2. Showing eigenvector plotted for eigenvector analysis of each critical principal component from Fig. 1. The high weight portions of each eigenvector are evaluated for their contribution in discriminating the sample sets.

7.2. Example 2

Nine tests are available for a variety of product B variations and its performance abilities under actual use conditions. PCA was again used to determine which tests indicated the highest correlation to high

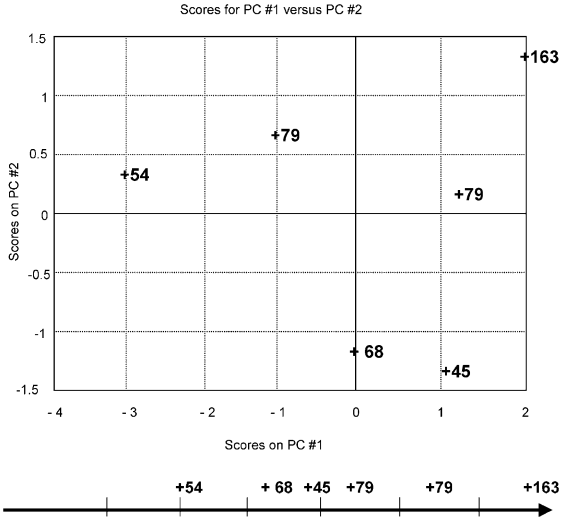

Fig. 3. Top: PCA scatter plot of multiple product test samples labeled with performance values. Specific attributes were determined to affect performance values. Bottom: Diagonal of PCA scatter plot showing product performance as a function of several definable attributes.

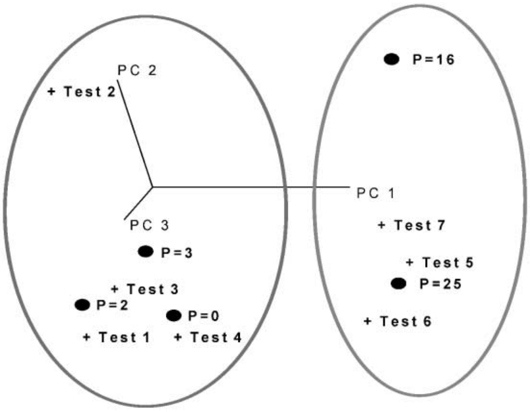

Fig. 4. PCA analysis of attributes and test results (scaled and overlaid for simultaneous viewing).

performance of product B. PCA discrimination was performed with successful interpretation of eigenvectors to determine optimum product B characteristics for performance (Fig. 3).

7.3. Example 3

Seven attribute tests were performed on product C and its physical performance measured. Each of the seven tests were believed to indicate a different characteristic of the product. Univariate review of the data by experts indicated no clear trends. PCA analysis clearly indicated three tests and a specific physical attribute indicated by these tests contributed to the physical performance of the product (Fig. 4).

8. Conclusion

In conclusion, eight basic, but powerful, principles might be derived from this discussion:

1. The commodity most lacking in today's NNE is human attention.
2. Value = Utility + Ubiquity.
3. A clear powerful message with results receives attention and communicates utility.
4. The easiest way to get the world using chemometrics is to solve their most urgent problems using the most parsimonious solutions.
5. Give these solution for free over the internet.
6. Once the value is noticed the techniques will proliferate more rapidly.
7. Then make more advanced tools and instruction available for solving data problems through standard commercial solutions.
8. Make web-based data and enhanced algorithms available for everyone (i.e., network the global PC community into chemometric—and multivariate—thinking).

The chemometrician is thus encouraged to apply multivariate thinking as a new means to problem solving for calibration and discovery. By applying multivariate problem-solving approaches to both analysis and discovery, an improvement in both the depth of discovery and the speed of discovery is possible. Solve urgent problems first using the simplest approach. Offer solutions to those who will cooperate in a network of discovery to provide ubiquity and synergy. Develop special tools and approaches to discovery that will lead to faster and more insightful work.

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