Angewandte

Advisory Board

The Seven Sins in Academic Behavior in the Natural Sciences

Wilfred F. van Gunsteren*

Scientific Best Practice

scientific best practice \cdot scientific misconduct \cdot scientific standards

n the high-technology societies of the twenty-first century scientists at academic institutions are often asked to explain or comment on complex technical issues that are of relevance to modern society and the common man. Members of academia are approached, as they are usually intelligent, highly knowledgeable, and honorable women and men, who are more faithful to scientific facts and truths than to themselves, their family or friends, or any organization in society. The role of academics as reliable and truthful messengers can only be maintained if academics are seen to adhere to the basic principles and rules of the academic scientific endeavor. However, with the rapid expansion in both the size and number of academic institutions over the past half century, the likelihood of scientists violating academic principles or espousing nonsense instead of truth is increasing. This is exemplified by the wave of plagiarism in the past decade that has been detected by the use of modern software and the recent case involving a highly publicized claim that particles had been detected moving faster than the speed of light, which was later retracted. While occurrences of deliberate scientific fraud are fortunately rare, whenever cases of inappropriate conduct go unchallenged and there is failure to maintain scientific standards, the trust that society bestows on academia will be undermined. That the German Secretary of Defense, Mr. zu Guttenberg, was forced to resign by a flood of emails from young scientists reminding the German Chancellor of the general importance of academic honesty should be seen as a highlight in the quest for scientific integrity.

What are the basic principles and rules of academic research? Academic research is primarily driven by curiosity, by the need to determine relationships between observations, and the desire to develop models that can be used to understand and predict phenomena in the world in which we live. Irrespective of one's intentions, one is easily fooled by flawed observations, missing, confounding variables, or incorrect assumptions. For this reason, any model or theory that is proposed must be justified and tested against data that are both tangible and publicly available. Only in this way may other scientists check the validity of a proposed model or theory without having to repeat the original work. Academic research is a continuous process of refinement. Every generation of researchers stands to some extent on the shoulders of those who have gone before. It is in this way that we advance our knowledge and understanding of the world.^[1] This basic tenet of academic endeavor in turn defines the fundamental requirements for effective research: clarity of presentation, reproducibility of data, testing of assumptions, search for additional variables, and the acknowledgement of both the ideas and the data used in the work but generated by others. The challenge is that these basic principles of highquality scientific research are increasingly in conflict with the mounting pressure placed on academic scientists to compete for grant money and to publish work continuously, in particular in so-called high-impact journals where sensationalism and potential publicity is often given more weight than scientific rigor. This in turn leads to inappropriate measures of success, which only serve to undermine the intrinsic value of scientific endeavor.

With respect to the violation of the basic rules of academic research one may distinguish seven "deadly sins". In order of increasing gravity these are:

- 1. A poor or incomplete description of the work, for example, publishing pretty pictures instead of evidence of causality.
- 2. Failure to perform obvious, cheap tests that could confirm or repudiate a model, theory, or measurement, for example, to detect additional variables or to show under which conditions a model or theory breaks down.
- 3. Insufficient connection between data and hypothesis or message, leading to lack of support for the message or over-interpretation of data, for example, rendering the story more sensational or attractive.
- 4. The reporting of only favorable results, for example, reporting positive or desired (hoped for) results while omitting those that are negative.
- 5. Neglect of errors found after publication.
- 6. Plagiarism.
- 7. The direct fabrication or falsification of data.

OTS adds: don't waste people's time by increasing the dimensionality of data merely for presentation purposes!

^[*] Prof. Dr. W. F. van Gunsteren Laboratory of Physical Chemistry Swiss Federal Institute of Technology, ETH, CH-8093 Zürich (Switzerland)

1. A Poor or Incomplete Description of the Work

Reproducibility is a critical element of good science. With the enhanced speed of computers, the increased complexity of experimental equipment, and the growth of the sophistication of the associated mathematical analysis aided by computers, the publication and analysis of all data required for others to reproduce the work has become more cumbersome. The pressure on journal space has led to such an erosion of this academic principle that the majority of work published in high-profile journals such as Science and Nature cannot be fully understood and reproduced based on the data published. Increasingly, pictures take precedence over data. Critical aspects of the methodology are not described. Instead, there is a trend towards the deposition of information in the form of supplementary material to papers. Generally, supplementary information leaves the impression of being less well described and reviewed than the main body of a paper. It must be said that striving for reproducibility is not as easy as it sounds, because the selection of parameter values crucial for the reproduction of the work is delicate. Failure to do so has also occurred in my own research publications. For example, in 2003 we tried to reproduce the density and heat of vaporization of a model for liquid dimethyl sulfoxide we had proposed in 1995,^[2] but we could not precisely reproduce the published values^[3] and explain the discrepancy, because some parameter values were missing in the original publication.

2<mark>. Failure to Perform Obvious, Cheap Tests that</mark> Could Confirm or Repudiat<mark>e a Model, Theory, or</mark> Measurement

All models or theories are an abstraction of reality and, as such, have limited applicability. This means that an essential element of any model is the conditions under which it is valid and knowledge of when it fails to properly describe a given phenomenon. In other words, an attempt to falsify a given model or theory by testing systematically the assumptions and parameters on which the model is based is an essential element of any publication of its characteristics. The observed correlations within a set of data that may have led to the particular model or theory should be tested so as to detect additional, confounding variables or the existence of alternative models or theories that may offer a better explanation of the observed correlations than the proposed model. Of course, such an investigation of alternative explanations or models has its limits with respect to the pecuniary or time effort required, but the simple, cheap tests ought to be conducted. The more extraordinary or significant the message or claim of a publication is, the more effort should be committed to such an investigation of its possible flaws. In the recent case where it had been claimed that particles had travelled faster than the speed of light,^[4] a result that would overturn one of the most basic premises of modern physics, the flaw in the results on which the claim was based was traced to a faulty cable.^[5] Interestingly, during the five months between the publication of the report stating that neutrinos could fly faster than light^[4] in September 2011 and its

retraction^[5] in February 2012 tens of theoretical physics papers were published with theories that allowed for particles moving faster than light.^[6]

3. Insufficient Connection between Data and Hypothesis or Message, Leading to Lack of Support for the Message or Over-Interpretation of Data

The plausibility of any scientific idea or hypothesis is dependent on the nature of the data used to support or validate it.^[7] In other words, it requires a critical analysis and interpretation of the data used that should establish an argument for the idea or hypothesis. It should be argued why these data are of relevance or provide support to the idea, hypothesis, or phenomenon. Often the data show trends that hint at a particular refinement of the model or explanation of a phenomenon that was not part of the original model or hypothesis, without providing sufficient statistics or support for it. Here interpretation is transformed into mild speculation which is useful to inspire readers to initiate research into the issue. However, pressure to publish exciting results in high-profile journals may seduce authors into over-interpretation or even wild speculation regarding their data, which is, in the absence of reproducibility, misleading. The fine art of interpreting data is to say no more but also no less than the data allow for.^[8] Yet, speculation is of course allowed, as long as it is presented as such. Academic research cannot do without imagination.

4. The Reporting of Only Favorable, Positive, or Desired Results

Because of the ever-increasing stream of scientific publications, editors of journals show a tendency to select for exciting, "new, or "positive" results that will attract the attention of a wide audience. This in turn induces a tendency for researchers to report only the wanted, hoped for, or "positive" results that will be well received by the research community, thereby sweeping the negative ones, in particular the tests not supporting the model or theory, under the rug. Needless to say, this tendency is deadly for the academic research endeavor, because it undermines the reliability of published results. With each new article published that supports a flawed model or theory it becomes increasingly difficult to overturn the model or theory. An example of selective publication is an article in the journal *Nature* on a simulation of the crystallization of water.^[9] The article implied that the crystallization occurred rapidly and spontaneously, whereas in reality it was a single rare event brought about by forcing the density of the liquid to equal that $\oint f$ the crystal. Reports of the failure to confirm a hypothesis or to reproduce data are as important scientifically as reports of success. Such reports not only help other researchers to avoid wasting time and effort on similar hypotheses, but are essential to scientific progress.





5. Neglect of Errors Found after Publication

Since academic research explores uncharted territory, erroneous observations and calculations, and other unintended errors are inevitable. One of the mechanisms to detect research errors is the publication of research in reproducible form. Failure to reproduce published results often leads to the detection, either by other research groups^[10] or by the authors themselves,^[11] of errors in the original work. In order to avoid the propagation of errors and the use of erroneous data in research, errors that are detected ought to be reported appropriately in the literature, either by an erratum or a corrigendum, or in a subsequent publication on the same topic. Failure to do so leads to unnecessary work by others. One could even defend the proposition that a scientist with a sizeable publication record in science who has not published a single corrigendum is unlikely to be a good scientist. Either he or she has done such simple work that nothing could go wrong, or he or she has committed the fifth sin in science.

6. Plagiarism

The nature of academic research, driven by curiosity and an urge to understand the world, thereby building on the knowledge and insights of preceding generations of scientists, does not allow for concepts such as ownership of ideas or data. In principle, one shares data and ideas in order to sharpen insights and avoid wasteful repetition. This principle though requires honesty about the origin of ideas and data. In other words, when research is presented, orally or in written form, the data and ideas of other researchers should be properly referenced. This is why plagiarism belongs to the sins in science. Proper referencing is not as simple as it sounds, because it requires judgement and the selection of data and ideas in order to avoid the useless referencing of all papers that are remotely related to the topic presented. Referencing should firstly involve data and ideas used or needed for reproducibility. Next it should be used to embed the topic of the research presented in a wider framework and to point the reader to related research.

Recently it has become a pastime of "witch hunters" to use software that can compare different documents available on the web in order to detect identical strings of text, which is then branded plagiarism. Identical text appearing in two published documents by different authors need not be an instance of plagiarism. In particular, technical descriptions of a procedure with slightly varying parameter values that is used in research over and over will not be changed from one paper to the next or from PhD thesis to PhD thesis, because there is no academic value in modifying a description already highly optimized with respect to clarity. Such copying of text does not violate the basic rules of academia and doesn't constitute plagiarism. In the same vein, it is no basic sin to copy one's own text. Moreover, to call such behavior selfplagiarism is a contradiction in terms. Yet, it is an accepted convention not to publish a report twice. When reporting their research orally though, scientists often repeat themselves giving the same presentation for substantially the same

audiences. In the education of students, repetition is even rather efficient. Repetition in written form though, while not a basic sin, constitutes annoying behavior that leads to a waste of effort by editors and reviewers and denigration of the literature. It may also involve the violation of a copyright, as is illustrated by the recent example of a story published in three different journals.^[12-14]

True plagiarism is, however, the theft of ideas followed by improper referencing. For example, quoting the original author of an idea only once in one's first paper on the topic and then further only quoting one's own paper, or during a presentation mentioning the author of an idea only when he or she happens to be present in the audience. Compared to this real plagiarism, simple copying of text is harmless.

Fortunately, the situation in the natural sciences with respect to plagiarism is less problematic than in the other branches of science, because in the former, researchers mostly describe results generated by themselves and not by others. Yet, it seems often difficult for authors of an idea, model, or method to publicly admit that someone else has had the same or a similar idea years before.

7. Fabrication or Falsification of Data

Fabrication or falsification of data is the worst sin in science, because it belies the fundamental value of trust between scientists who, when exploring new territory, must be able to count on the honesty of their fellows. The cases of fabrication of data, for example in physics,^[15] biology,^[16] and chemistry,^[17,18] are relatively rare, fortunately, and it is gratifying that a case was uncovered even 10 years after the original publication.^[17,18] Although it is impossible to avoid such cases altogether, because one cannot check all the data generated by a student or researcher, academic scientists should strive for working habits that will reduce the risk of falling prey to the fabrication of data.

What Can Be Done by Whom To Safeguard the Basic Principles of Academic Research?

Within a research group the principal investigator should pay attention to the elucidation of the basic principles of academic research and the seven sins. He or she should create conditions that prevent missteps in conduct: working habits that allow for repeating each other's experiments or calculations, a group atmosphere that makes it easy to admit error and that fosters a critical discussion of results, and a reluctance to publish data too rapidly for a thorough checking for possible flaws.

Editors of journals should focus less on the news value and smallest possible page-count of a manuscript than on its intrinsic quality: Is it clearly written? Are the data reproducible? Is the data or message new and contributing significantly to scientific knowledge? Is the message supported by the data? Data in the form of tables and figures are of more use to a reader who wants to draw his or her own conclusions from the data than the interpreting text written by an author. Second, editors should avoid the service of reviewers who abuse their reviewing function to impose their own views upon another scientist's manuscript, or who use their reviewing function to generate citations.^[19] Third, editors should allow for the concise reporting of negative results, because a research journal is not a newspaper, but rather a repository or databank of research ideas and knowledge.

Administrative officials at universities and other academic institutions should refrain from issuing detailed regulations that may stifle the creativity and adventurism on which research depends.^[20] They should rather foster discussion about basic principles and appropriate behavior, and judge their staff and applicants for jobs based on their curiositydriven urge to do research, understand, and share their knowledge rather than on superficial aspects of academic research such as counting papers or citations or considering a person's grant income or h-index or whatever ranking, which generally only reflect quantity and barely quality. If the curriculum vitae of an applicant lists the number of citations or an h-index value or the amount of grant money gathered, one should regard this as a sign of superficiality and misunderstanding of the academic research endeavor, a basic flaw in academic attitude, or at best as a sign of bad taste.

Politicians should recognize that artificial competition for financial support for investigators or universities based on indices or rankings, that is, on one-dimensional projections of an almost infinitely dimensional activity or organization, will not only lead to ever more bureaucracy and other unwanted side effects such as increasingly useless publications,^[21] but will also destroy academic values such as carefulness, willingness to share results, and honesty.

Finally, I would cite from the work of Tony Judt,^[22] who in an essay about his time as a student at King's College, Cambridge, UK writes: "College teaching was idiosyncratic. Most of my supervisors—John Saltmarsh, Chistopher Morris, and Arthur Hibbert-were obscure, published little, and known only to generations of Kingsmen. Thanks to them I acquired not just a patina of self-confidence, but abiding respect for teachers who are *indifferent to fame (and fortune)* and to any consideration outside the supervision armchair. We were never taught with the specific aim of performing well on the Tripos-the Cambridge final examinations. My supervisors were supremely uninterested in public performance of any sort. It was not that they were indifferent to exam results; they simply took it for granted that our natural talent would carry us through. It's hard to imagine such people today, if only because they would be doing the college a profound disservice in the face of the Research Assessment Exercise, whereby the British government assesses "academic output" and disburses funds accordingly."

In the year 1770 the Anglo-Irish writer and poet Oliver Goldsmith wrote a pastoral poem of 430 lines,^[23] of which lines 51 and 52 read:

"Ill fares the land, to hastening ills a prey,

where wealth accumulates and men decay".

Transposed to the academic research endeavor one might declare:

"Ill fares the university, to hastening ills a prey,

where status and window dressing accumulate, curiosity and honesty decay".

I thank Jane Allison, Jožica Dolenc, Peter Gölitz, David Gugerli, Don Hilvert, Philippe Hünenberger, Alan Mark, Frédéric Merkt, Roel Prins, and Sereina Riniker for helpful comments and suggestions.

Received: July 25, 2012 Published online: December 3, 2012

- R. K. Merton, On the Shoulders of Giants: A Shandean Postscript: The Post-Italianate Edition (with Umberto Eco and Denis Donoghue), University of Chicago Press, Reprint Edition, 1993, ISBN 0-226-52086-2.
- [2] H. Liu, F. Müller-Plathe, W. F. van Gunsteren, J. Am. Chem. Soc. 1995, 117, 4363–4366.
- [3] D. P. Geerke, C. Oostenbrink, N. F. A. van der Vegt, W. F. van Gunsteren, J. Phys. Chem. B 2004, 108, 1436–1445.
- [4] T. Adam, N. Agafonova, O. Altinok, P. Alvarez Sanchez, S. Aoki, T. Ariga, D. Autiero, C. Bozza, T. Brugière, R. Brugnera, F. Brunet, G. Brunetti, S. Buontempo, B. Carlus, F. Cavanna, G. Colosimo, N. D'Ambrosio, G. De Lellis, Y. Déclais, P. del Amo Sanchez, F. Di Capua, D. Di Ferdinando, N. Di Marco, S. Dmitrievsky, D. Duchesneau, S. Dusini, I. Efthymiopoulos, O. Egorov, T. Ferber, R. A. Fini, T. Fukuda, G. Giacomelli, C. Girerd, C. Göllnitz, et al. (122 additional authors not shown), Measurement of the neutrino velocity with the OPERA detector in the CNGS beam, arXiv:1109.4897v2.
- M. Antonello, P. Aprili, B. Baiboussinov, M. Baldo Ceolin, P. [5] Benetti, E. Calligarich, N. Canci, S. Centro, A. Cesana, K. Cieślik, D. B. Cline, A. G. Cocco, A. Dabrowska, D. Dequal, A. Dermenev, R. Dolfini, C. Farnese, A. Fava, A. Ferrari, G. Fiorillo, D. Gibin, A. Gigli, Berzolari, S. Gninenko, A. Guglielmi, M. Haranczyk, J. Holeczek, A. Ivashkin, J. Kisiel, I. Kochanek, J. Lagoda, S. Mania, G. Mannocchi, A. Menegolli, G. Meng, C. Montanari, S. Otwinowski, L. Periale, A. Piazzoli, P. Picchi, F. Pietropaolo, P. Plonski, A. Rappoldi, G. L. Raselli, M. Rossella, C. Rubbia, P. Sala, E. Scantamburlo, A. Scaramelli, E. Segreto, F. Sergiampietri, D. Stefan, J. Stepaniak, R. Sulej, M. Szarska, M. Terrani, F. Varanini, S. Ventura, C. Vignoli, H. G. Wang, A. Zalewska, K. Zaremba, P. Alvarez Sanchez, J. Serrano; Measurement of the neutrino velocity with the ICARUS detector at the CNGS beam, arXiv:1203.3433.
- [6] http://de.arXiv.org.
- [7] W. F. van Gunsteren, A. E. Mark, J. Chem. Phys. 1998, 108, 6109-6116.
- [8] W. F. van Gunsteren, J. Dolenc, A. E. Mark, Curr. Opin. Struct. Biol. 2008, 18, 149–153.
- [9] M. Matsumoto, S. Saito, I. Ohmine, Nature 2002, 416, 409-413.
- [10] C. D. Christ, W. F. van Gunsteren, J. Chem. Phys. 2008, 128, 174112; Erratum: C. D. Christ, W. F. van Gunsteren, J. Chem. Phys. 2011, 134, 229901.
- [11] M. Christen, A.-P. E. Kunz, W. F. van Gunsteren, *J. Phys. Chem. B* 2006, *110*, 8488–8498; Erratum: M. Christen, A.-P. E. Kunz, W. F. van Gunsteren, *J. Phys. Chem. B* 2008, *112*, 11446.
- [12] R. Breslow, Tetrahedron Lett. 2011, 52, 4228-4232.
- [13] R. Breslow, Isr. J. Chem. 2011, 51, 990–996.
- [14] R. Breslow, J. Am. Chem. Soc. 2012, 134, 6887-6892.
- [15] M. R. Beasley, S. Datta, H. Kogelnik, and H. Kroemer, Report of the Investigation Committee on the Possibility of Scientific Misconduct in the Work of Hendrik Schoen and Coauthors, September 2002, (pdf), Bell Labs, http://en.wikipedia.org/wiki/ Sch%C3%B6n_scandal#References.



- [16] W. S. Hwang, Y. J. Ryu, J. H. Park, E. S. Park, E. G. Lee, J. M. Koo, H. Y. Jeon, B. C. Lee, S. K. Kang, S. J. Kim, C. Ahn, J. H. Hwang, K. Y. Park, J. B. Cibelli, S. Y. Moon, *Science* 2004, *303*, 1669–1674; retracted: W. S. Hwang, Y. J. Ryu, J. H. Park, E. S. Park, E. G. Lee, J. M. Koo, H. Y. Jeon, B. C. Lee, S. K. Kang, S. J. Kim, C. Ahn, J. H. Hwang, K. Y. Park, J. B. Cibelli, S. Y. Moon, *Science* 2006, *311*, 335.
- [17] A. Pfaltz, W. F. van Gunsteren, M. Quack, W. Thiel, D. A. Wiersma, An Investigation with respect to the Possible Fabrication of Research Data reported in the Thesis ETH No 13629 and in the Papers Journal of Chemical Physics 112 (2000) 2575 and 113 (2000) 561, July 2009, ETH, http://www.ethlife.ethz.ch/ archive_articles/120123_Expertenbericht_tl/120123_ Expertenbericht
- [18] A. Pfaltz, W. F. van Gunsteren, M. Quack, W. Thiel, D. A. Wiersma, An Investigation with respect to the Possible Fabrication of Research Data reported in the Thesis ETH No. 13629 and in the Papers Journal of Chemical Physics 112 (2000) 2575 and 113 (2000) 561, Appendices, July 2009, ETH, http://www. ethlife.ethz.ch/archive_articles/120123_Expertenbericht_tl/ 120123_Expertenbericht_Anhange.
- [19] J. Reedijk, Angew. Chem. 2012, 124, 852–854; Angew. Chem. Int. Ed. 2012, 51, 828–830.
- [20] G. Schatz, FEBS Lett. 2003, 553, 1-2.
- [21] M. Binswanger, Sinnlose Wettbewerbe: Warum wir immer mehr Unsinn produzieren, Herder, Freiburg im Breisgau, 2010.
- [22] T. Judt, The Memory Chalet, Vintage Books, London, 2011.
- [23] *The Complete Poetical Works of Oliver Goldsmith* (Ed.: H. Austin Dobson), ISBN 1-58827-277-X.