Preface

An analyst working in an analytical laboratory today is not only expected to understand their instrumental methods and the chemistry of their test materials and analytes. They are also expected to understand and to follow basic principles of good practice in analytical measurement. One summary of these is the set of six principles currently disseminated by the Chemical and Biological Metrology Programme (see http://www.nmschembio.org.uk for details):

- *Principle 1:* Analytical measurements should be made to satisfy an agreed requirement.
- *Principle 2:* Analytical measurements should be made using methods and equipment which have been tested to ensure they are fit for purpose.
- *Principle 3:* Staff making analytical measurements should be both qualified and competent to undertake the task.
- *Principle 4:* There should be a regular independent assessment of the technical performance of a laboratory.
- *Principle 5:* Analytical measurements made in one location should be consistent with those elsewhere.
- *Principle 6:* Organisations making analytical measurements should have well-defined quality control and quality assurance procedures.

Of these, Principle 1 is usually identified with the procedures of contract review, planning and selection of methods and sampling protocols, Principle 2 with method validation, Principle 3 with proper education, training and qualification of analytical staff, Principle 4 with regular proficiency testing (PT), Principle 5 with the establishment of traceability through calibration of equipment and Principle 6 with the implementation of appropriate analytical quality assurance (QA) and quality control (QC) procedures, typically backed up by formal accreditation or other third-party assessment of quality systems.

Although there is much more to this than statistics, effective use of statistical methods certainly has a role in many of these processes. Method development and validation obviously depend very heavily on statistical methods, both for the design of suitable experiments and for the statistical tests used to identify problems and improvements and to confirm acceptability. Calibration of instruments almost invariably uses statistical methods, particularly least-squares regression. Proficiency testing organisers use statistical methods to summarise participant data and calculate scores and the interpretation of PT scores within a laboratory relies on basic statistical techniques and concepts. In sampling, the idea of a 'representative sample' is itself a statistical concept and proper sampling is fundamental; no analytical measurement is better than the sample analysed, and

Practical Statistics for the Analytical Scientist: A Bench Guide, 2nd Edition
Stephen L R Ellison, Vicki J Barwick, Trevor J Duguid Farrant

Published by the Royal Society of Chemistry, www.rsc.org

deciding on the appropriate number and type of test items is a key part of planning in many analytical projects. Day-to-day analytical quality control is also heavily dependent on statistical methods. It is no surprise, then, that third-party assessors invariably look for a sound statistical basis for all of these processes. This book is therefore intended to help analytical scientists use statistics effectively in their day-to-day work.

The first edition was written as a bench manual, covering the basic statistics needed in an analytical laboratory and providing detailed calculations for many of the more common operations. This second edition is a very substantial revision of the first. The changes have three principal causes. First, we wished to take advantage of the revision to improve the clarity and authority of the text, essentially all of which has been revised. In the process, we have added references to the principal literature sources for many tests and reviewed and amended many of the statistical procedures and the reference data. The Grubbs and Dixon tables in particular have been updated to follow recent published implementations and we have reverted to Grubbs' original implementation of Grubbs test 3 for greater consistency with other texts. The interpretation of two-way ANOVA has also been amended significantly, largely to allow valid interpretation irrespective of whether the effects under study are random or fixed.

Second, there have been significant changes in the availability of statistical software. Essentially every analytical scientist now has access to software for common statistical operations, including *t*-tests, regression and analysis of variance, even if only the implementations in common spreadsheet software. Because of this, the text has been revised to concentrate on the interpretation of output from the calculations, rather than on the calculations themselves. The calculations are included for reference, but are now to be found in appendices rather than in the body text.

Third, we wished to add new material. A new chapter on graphical assessment of data reflects the importance of visual review and interpretation, an essential step in data analysis. Experimental design is covered in another entirely new chapter, covering the basics of experimental design and planning and introducing some of the more advanced experimental designs to be found in specialist software. Analytical QA practices now routinely include the topic of measurement uncertainty; another new chapter therefore provides a summary of uncertainty estimation procedures, key references and a comparatively simple methodology for practical use. A new chapter on method validation explains the application of basic statistical methods and experimental design to method validation studies. These join existing chapters on proficiency testing and sampling, also important parts of analytical QA.

The text has been restructured with the aim of making sections easier to find and to provide additional explanation and guidance, both in the body of the text and, for example, in the extended section on distributions and types of data. Examples in the body text have also been rewritten using experimental data wherever possible and the exercises revised and expanded to cover the new topics.

As before, the book is intended primarily as a reference to useful procedures, rather than a theoretical textbook. The Introduction is intended as the starting point, providing cross-references to the procedures necessary for common analytical tasks. Wherever possible in the main text, topics describe a step-by-step procedure for implementing the necessary procedures. Finally, the question section provides exercises and fully worked answers to cover all the applications, so that a newcomer can check their understanding before applying the procedures to their own data.

S L R Ellison
V J Barwick