Michael Grabe

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With 47 Figures

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To the memory of my parents

in love and gratitude

Preface

In his treatises on the Method of Least Squares C.F. Gauß [1] distinguished irregular or random errors on the one hand and regular or constant errors on the other. As is well known, Gauß excluded the latter from his considerations on the ground that the observer should either eliminate their ultimate causes or rid every single measured value of their influence.

Today, these regular or constant errors are called unknown systematic errors or, more simply, systematic errors. Such errors turned out, however, to be eliminable neither by appropriately adjusting the experimental set-ups nor by any other means. Moreover, considering the present state of measurement technique, they are of an order of magnitude comparable to that of random errors.

The papers by C. Eisenhart [9] and S. Wagner [10] in particular have entrusted the high-ranking problem of unknown systematic errors to the metrological community. But it was not until the late 1970s, that it took center stage apparently in the wake of a seminar held at the Physikalisch-Technische Bundesanstalt in Braunschweig [19]. At that time, two ways of formalizing unknown systematic errors were discussed. One of these suggested including them smoothly via a probabilistic artifice into the classical Gaussian calculus, and the other, conversely, proposed generalizing that formalism in order to better bring their particular features to bear.

As the author prefers to see it, systematic errors introduce biases, and this situation would compel the experimenter to differentiate between expectations on the one hand and true values on the other – a distinction that does not exist in the conventional error calculus. This perspective and another reason, which will be explained below, have induced the author to propose a generalization of the classical error calculus concepts. Admittedly, his considerations differ substantially from those recommended by the official metrology institutions. Today, the latter call for international validity under the heading *Guide to the Expression of Uncertainty in Measurement* [34–36].

Meanwhile, both formal and experimental considerations have raised numerous questions: The *Guide* does not make a distinction between true values and expectations; in particular, uncertainty intervals are not required to localize the true values of the measurands. Nonetheless, physical laws in general as well as interrelations between physical constants in particular are to be

expressed in terms of true values. Therefore, a metrology which is not aimed at accounting for a system of true values is scarcely conceivable.

As the *Guide* treats random and systematic errors in like manner on a probabilistic basis, hypothesis testing and analysis of variance should remain valid; in least squares adjustments, the minimized sum of squared residuals should approximate the number of the degrees of freedom of the linear system. However, all these assumptions do not withstand a detailed analysis.

In contrast to this, the alternative error model to be discussed here suggests healing answers and procedures appearing apt to overcome the said difficulties.

In addition to this, the proposal of the author differs from the recommendations of the *Guide* in another respect, inasmuch as it provides the introduction of what may be called "well-defined measurement conditions". This means that each of the measurands, to be linked within a joint error propagation, should be subjected to the same number of repeat measurements. As obvious as this might seem, the author wishes to boldly point out that just this procedure would return the error calculus back to the womb of statistics which it had left upon its way through the course of time. Well-defined measurement conditions allow complete empirical variance–covariance matrices to be assigned to the input data and this, in fact, offers the possibility of expressing that part of the overall uncertainty which is due to random errors by means of Student's statistics.

Though this idea is inconsistent with the traditional notions of the experimenters which have at all times been referred to incomplete sets of data, the attainable advantages when reformulating the tools of data evaluation in terms of the classical laws of statistics appear to be convincing.

There is another point worth mentioning: the approach to always assess the true values of the measurands in general and the physical constants in particular eliminates, quasi by itself, the allegedly most fundamental term of metrology, namely the so-called "traceability". Actually, the gist of this definition implies nothing else but just that what has been stated above, namely the localization of true values. While the *Guide* cannot guarantee "traceability", this is the basic property of the alternative error model referred to here.

Last but not least, I would like to express my appreciation of my colleagues' experience, which I referred to when preparing the manuscript as well, as their criticism, which inspired me to clarify the text. For technical support I am grateful to Dr. Michael Weyrauch and to Dipl.-Übers. Hannelore Mewes.

Braunschweig, January 2005 *Michael Grabe*

Contents

Part I

Characterization, Combination and Propagation of Errors

1 Basic Ideas of Measurement

1.1 Sources of Measurement Uncertainty

To measure is to compare. To this end, as we know, a well defined system of physical units is needed. As to the latter, we have to distinguish between the definitions and the realizations of units. By its very nature, a defined unit is a faultless, theoretical quantity. In contrast, a realized unit has been produced by a measuring device and is therefore affected by imperfections. Moreover, further errors occur when a realized unit is used in practice, as the comparison of a physical quantity to be measured with the appropriate unit is a source of measurement errors.

Let us assign a true value to every quantity to be measured or a measurand. True values will be indexed by a 0 and measured values by natural numbers $1, 2, \ldots$.[1] If x designates the physical quantity considered, then the symbols x_0, $x_1, x_2, \ldots$ denote the true value and the measured values.

To reduce the influence of measurement errors, it suggests to repeat the measurement, say n times, under the same conditions and to subsequently condense the set of repeat measurements thus gained to an estimator for the unknown (and unknowable) true value. Spontaneously one might wish n to be as large as possible hoping to achieve high measurement accuracy. However, there are limits to this wishful thinking.

A large number of repeat measurements would be meaningful only if the resolution of the measuring device is sufficiently high. If the resolution is low, it should hardly make sense to pick up a huge number of repeated measurements, as a coarse device will respond to one and the same quantity, repeatedly input, with a rather limited number of different output values.

To be more specific, the accuracy of measuring instruments suffers from random errors, which we are all familiar with, as well as from so-called unknown systematic errors, the knowledge of which appeared to be confined, at least until the late 1970s, to, say, esoteric circles. Unknown systematic errors remain constant in time and unknown with respect to magnitude and sign. Traditionally, they are not considered on the part of the classical Gaussian error calculus. As there is no chance of ignoring or eliminating such per-

[1] As a zeroth measurement does not exist, the index 0 in x_0 clearly distinguishes the true value from the measured data $x_1, x_2, \ldots$.

turbations, experimenters rather have to lock them within intervals of fixed extensions, the actual lengths of which have to be taken from the knowledge of the measuring devices and the conditions under which they operate.

Given that the unknown systematic errors as well as the statistical properties of the random process, which produces the random measurement errors, remain constant in time, the experimental set-up corresponds, put in statistical terms, to a stationary process. For the experimenter, this would be the best he can hope for, i.e. this would be, by definition, a perfect measuring device. Over longer periods, however, measuring devices may change their properties, in particular, unknown systematic errors may be subject to drifts.

In case unknown systematic errors changed following some trend, the measurements constitute something of the kind of a time series which would have to be treated and analyzed according to different methods which will be of no concern here.

As drifts might always occur, the experimenter should try to control the measurement conditions so that the unknown systematic errors remain constant at least during the time it takes to pick up a series of repeat measurements, say, $x_1, x_2, \ldots, x_n$, and to specify the extensions of the intervals confining the unknown systematic errors such that their actual values are always embraced.

After all, smaller samples of measured values may appear more meaningful than larger ones. In particular, averaging arbitrarily many repeat measurements, affected by time-constant unknown systematic errors, would not reduce the latter.

The true value of the physical quantity in question is estimated by means of a suitably constructed estimator. The experimenter should declare how much the two quantities, the true value and the estimator, might deviate from each other. The quantity accounting for the difference is called the measurement uncertainty. This basic quantity grants us access to the possible locations of the true value of the measurand relative to its estimator, Fig. 1.1.

As we do not know whether the estimator is larger or smaller than the true value – if we knew this, we would have disregarded executable corrections – we shall have to resort to symmetrical uncertainty intervals. Due to formal reasons, the numerical values of uncertainties are always positive quantities which we afterwards have to provide with a $\pm$ sign. We state:

The interval

$$\textit{estimator} \pm \textit{measurement uncertainty}$$

defines the result of a measurement. This range is required to localize the true value of the measurand (or quantity to be measured).

As a rule, measurement uncertainties will be composed of two parts, one is due to random errors and the other is due to unknown systematic errors.

In this context, the terms accuracy and reproducibility turn out to be crucial, see also Sect. 4.1. The accuracy refers to the localization of the true

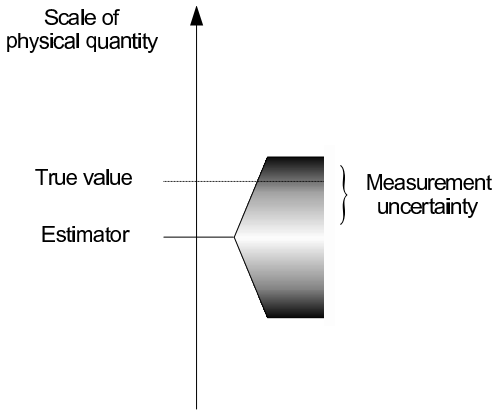


Fig. 1.1. The interval (estimator ± measurement uncertainty) is required to localize the true value of the measurand

value of the measurand: The smaller the uncertainty the higher the accuracy. In contrast to this, reproducibility merely aims at the statistical scattering of the measured data: The closer the scattering the higher the reproducibility.

Obviously, it is neither necessary nor advisable to always strive for highest attainable accuracies. But, in any case, it is indispensable to know the actual accuracy of the measurement and, in particular, that the latter reliably localizes the true value. The national metrology institutes ensure the realization of units by means of hierarchies of standards. The respective uncertainties are clearly and reliably documented so that operators can count on them at any time and at any place.

In the natural sciences, a key role comes to measurement uncertainties as principles of nature are verified or rejected by comparing theoretical predictions with experimental results. Here, measurement uncertainties have to decide whether new ideas should be accepted or discarded.

In engineering sciences measurement uncertainties provide an almost unlimited diversity of intertwined dependencies which, in the end, are crucial for the functioning, quality, service life and competitiveness of industrial products.

Trade and industry categorically call for mutual fairness: both, the buyer and the seller expect the measuring processes to so subdivide merchandise and goods that neither side will be overcharged.[2]

Figure 1.2 sketches the basics of a measuring process. The construction of a measuring device will be possible not until the physical model has found a mathematical formulation. After this, procedures for the evaluation of the

[2]One might wish to multiply the relative uncertainties (defined in (1.2) below) of the counters for gas, oil, petrol and electricity by their annual throughput and the respective prices.

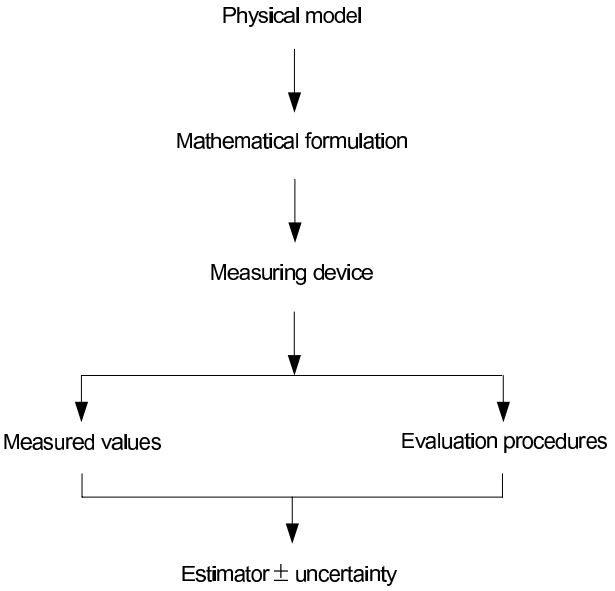


Fig. 1.2. Diagram of a measuring process

measurements have to be devised. As a rule, the latter require additional assumptions, which are either independent of the measuring process, such as the method of least squares, or depend on it such as, for example, the statistical distribution of random errors and the time-constancy of unknown systematic errors. The monograph at hand confines itself to estimators whose structures are that of unweighted or weighted arithmetic means. Whether or not the procedures estimating their measurement uncertainties may be transferred to estimators satisfying other criteria will not be discussed here.

Let any given arithmetic mean $\bar{x}$ and its uncertainty $u_{\bar{x}} > 0$ have, after all, been estimated. Then, the mathematical notation will be

$$\bar{x} \pm u_{\bar{x}}\,. \tag{1.1}$$

Example

Let

$$\bar{m} \pm u_{\bar{m}} = (10.31 \pm 0.05)\,\mathrm{g}$$

be the result of a weighing. Then the true value m_0 of the mass m is required to lie somewhere within the interval $10.26\,\mathrm{g},\ldots,10.36\,\mathrm{g}$.

The uncertainty $u_{\bar{x}}$ may be used to derive other, occasionally useful, statements. In this sense, the quotient

$$\frac{u_{\bar{x}}}{\bar{x}} \tag{1.2}$$

denotes the relative uncertainty. Herein, we might wish to substitute x_0 for $\bar{x}$. This, however, is prohibitive, as the true value is not known. Relative uncertainties vividly illustrate the accuracy of measurement, independent of the order of magnitude of the respective estimators. Let U_1 and U_2 designate any physical units and let

$$\bar{x}_1 = 10^{-6}\,\mathrm{U}_1\,, \quad \bar{x}_2 = 10^{6}\,\mathrm{U}_2$$

be estimators with the uncertainties

$$u_{\bar{x}_1} = 10^{-8}\,\mathrm{U}_1\,, \quad u_{\bar{x}_2} = 10^{4}\,\mathrm{U}_2\,.$$

The two estimators have, obviously, been determined with equal accuracy, though their uncertainties differ by not less than 12 decimal powers.

There are uncertainty statements which are still more specific. The frequently used ppm uncertainty (ppm means "parts per million") makes reference to the decimal power of 6. The quotient

$$\frac{u_{\bar{x}}}{\bar{x}} = \frac{u_{\mathrm{ppm}}(\bar{x})}{10^6}$$

thus leads to

$$u_{\mathrm{ppm}}(\bar{x}) = \frac{u_{\bar{x}}}{\bar{x}} 10^6\,. \tag{1.3}$$

The idea is to achieve a more comfortable notation of numbers by getting rid of decimal powers which are known a priori. As an example, let $u_{\mathrm{ppm}} = 1$; this implies $u_{\bar{x}}/\bar{x} = 10^{-6}$.

Example

The frequency ν of the inverse ac Josephson effect involves dc voltage steps $U = (h/2e)\nu$; e designates the elementary charge and h the Planck constant. Let the quotient $2e/h$ be quantified as

$$4.8359767(14)\,10^{14}\,\mathrm{Hz\,V^{-1}}\,.$$

How is this statement to be understood? It is an abbreviation and means

$$2\overline{e/h} \pm u_{\overline{2e/h}} = (4.8359767 \pm 0.0000014)10^{14}\,\mathrm{Hz\,V^{-1}}\,.$$

Converting to ppm yields

$$u_{\mathrm{ppm}} = \frac{0.0000014 \cdot 10^{14}\,\mathrm{Hz\,V^{-1}}}{4.8359767 \cdot 10^{14}\,\mathrm{Hz\,V^{-1}}} \cdot 10^6 = 0.289\ldots$$

or, rounding up,

$$u_{\mathrm{ppm}}(2\overline{e/h}) = 0.30\,.$$

1.2 Quotation of Numerical Values and Rounding

Evaluation procedures nearly always endow estimators with dispensable, insignificant decimal digits. To get rid of them, the measurement uncertainty should tell us where and how we have to round and, in particular, how to quote the final result [37].

1.2.1 Rounding of Estimators

First of all, we determine the decimal place in which the estimator should be rounded. Given that the first decimal of the measurement uncertainty differing from 0 turns out to be one of the digits

$$\left.\begin{array}{r}1\text{ or }2\\ \\ 3\text{ up to }9\end{array}\right\}\quad\text{the estimator should be rounded}\quad\left\{\begin{array}{c}\text{in the place to the right}\\ \text{of this place}\\ \\ \text{in just this place}\end{array}\right.$$

Having determined the decimal place of the estimator in which it should get rounded, we round it

$$\left.\begin{array}{r}\text{down,}\\ \text{up,}\end{array}\right\}\quad\begin{array}{l}\text{if the decimal place to the right}\\ \text{of this place is one of the digits}\end{array}\quad\left\{\begin{array}{l}0\text{, up to }4\\ 5\text{, up to }9\end{array}\right.$$

1.2.2 Rounding of Uncertainties

The uncertainty should be rounded up in the decimal place in which the estimator has been rounded.

Sometimes the numerical value of a physical constant is fixed with regard to some necessity. It goes without saying that fixing a physical constant does not produce a more accurate quantity. A possibility to emphasize a fixed digit would be to print it boldly, e.g. 273.1**6** K.

Table 1.1. Rounding of estimators and uncertainties

raw results			rounded results		
5.755018 ...	±	0.000194 ...	5.75502	±	0.00020
1.9134 ...	±	0.0048 ...	1.913	±	0.005
119748.8 ...	±	123.7 ...	119750	±	130
81191.21 ...	±	51.7 ...	81190	±	60

Examples

Let

$$(7.238143 \pm 0.000185)\,\mathrm{g}$$

be the result of a weighing. The notation

$$\begin{array}{l} 7\,.\,2\,3\,8\,1\,4\,3 \\ \qquad\qquad\uparrow \\ 0\,.\,0\,0\,0\,1\,8\,5 \end{array}$$

facilitates the rounding procedure. The arrow indicates the decimal place in which the estimator should be rounded down. In just this decimal place the uncertainty should be rounded up, i.e.

$$(7.23814 \pm 0.00019)\,\mathrm{g}$$

For simplicity, in the examples presented in Table 1.1 the units will be suppressed.

2 Formalization of Measuring Processes

2.1 Basic Error Equation

Measuring instruments are known to not operate perfectly. Nevertheless, for the experimenter it suffices to register a sequence of repeat measurements of, say, n outcomes

$$x_1, x_2, \ldots, x_n \,, \tag{2.1}$$

which are free from drift. Obviously, under these circumstances, the data will scatter around a horizontal line, Fig. 2.1. As Eisenhart [9] has vividly formulated, the measuring instrument then operates in a state of statistical control. Then, as we shall assume, the measurement errors may be subdivided in two classes, namely in

- random errors and
- unknown systematic errors,

the latter being constant in time, at least during the period it takes to carry out the measurements.

The reservation "during the period of measurement" is essential as it may well happen that when repeating the measurements at a later time, the systematic errors may assume other values, giving rise to a different stationary state. To that effect, the boundaries of the unknown systematic errors should be fixed such that they encompass, once and for all, all potential realizations of the systematic errors.

Any drift, however, would model the data according to some trend. The measuring process would then no longer be stationary and instead of a "horizontally" scattering series of repeated measurements, the experimenter would have registered something similar to a time series.

There will certainly be no drifts, if the so-called influence quantities of the measuring process remain constant in time. Those latter quantities are related to environmental and boundary conditions, to the thermal and mechanical stability of the experimental set-up, to the stability of its detectors, its power supplies, etc.

Generally speaking, a non-drifting measuring device will not be free from systematic errors as the absence of drifts rather merely means that the influences of systematic perturbations are invisible – just on account of their constancy.

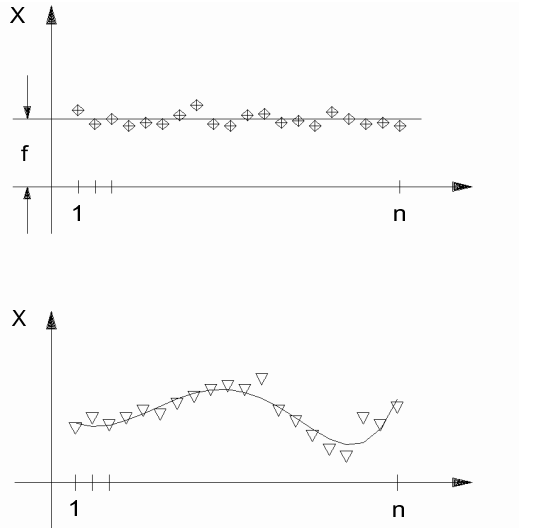


Fig. 2.1. Non-drifting (above) and drifting (below) sequences of repeated measurements

While random errors occur instantaneously, in the course of the measurements, the actual values of systematic errors are predetermined before the measurements get started.

In theoretical terms, systematic errors arise when physical models are conceptualized as, in general, this calls for approximations and hypotheses. At an experimental level, systematic errors may be due to inexact adjustments and pre-settings, to environmental and boundary conditions, which are known to be controllable only with finite accuracy, etc. As an example, let us consider the density of air. Though its values appear to be predictable with remarkable accuracy, there still remains a non-negligible uncertainty component which is due to unknown systematic errors. In weighings of high accuracy, the greater the differences between the densities of the masses to be compared, (e.g. platinum-iridium 21 500 $\mathrm{kg/m^3}$ and steel 8 000 $\mathrm{kg/m^3}$), the greater the uncertainty of the correction due to air buoyancy. As operators complain, this latter uncertainty, unfortunately, makes a significant contribution to the overall uncertainty of the weighing [26].

Furthermore, the switching-on of an electrical measuring device will not always lead to one and the same stationary state, and the same applies to the use of a mechanical device. Last but not least, inherently different procedures for measuring one and the same physical quantity will certainly bring about different systematic errors [14].

Random errors have to be attributed to microscopic fluctuations of events which affect the measuring process and prove to be uncontrollable on a macroscopic scale. According to experience, the random errors of stationary exper-

imental set-ups may be considered, at least in reasonable approximation, to follow a normal probability distribution. Though we are not in a position to understand these phenomena in detail, we find guidance in the central limit theorem of statistics [43]. According to this, loosely stated, the superposition of sufficiently many similar random perturbations tends to a normal distribution.

Actually, for practical reasons, the statistical properties of measured data are rarely scrutinized. Nevertheless, we have to declare: should the assumption of normally distributed data fail, the procedures for the estimation of the random part of the overall measurement uncertainties, outlined in the following step by step, will not apply.

The status of unknown systematic errors is quite different. First of all, the question as to whether or not they should be treated probabilistically is still controversial [10,19]. Though the measuring process as outlined above relates them to a probabilistic origin, this is not meant in the sense of repeatable events but with respect to the observation that the experimenter has no chance of controlling or influencing the chain of events which, in the end, leads to an operative systematic error. Again, while it is true that systematic errors have their roots in random events, on account of their constancy, and in order to arrive at reliable measurement uncertainties, we prefer to treat them non-probabilistically and make allowance for them by introducing biases and worst-case estimations. We might say that the approach of the *Guide* to randomize unknown systematic errors corresponds to an a priori attitude, whereas the idea to classify them as biases reflects an a posteriori position. While the former roots in theoretical considerations, the latter starts from experimental facts.

Should there be just one systematic error, it should certainly not be difficult to draw indisputable conclusions. Yet, it will be more controversial to assess the influence of several or even many unknown systematic errors. We shall discuss this situation in Sects. 2.3 and 6.3.

As is common practice, we let f denote the unknown systematic error and let

$$f_1 \leq f \leq f_2\,; \quad f = \text{const.}$$

specify the confining interval. We expect the boundaries f_1 and f_2 to be safe, which simply means that f shall not lie outside the limits. As banal as this might sound, just as little should we forget that a declaration of intent is one matter and its implementation another. To recognize the sources of systematic errors, to formalize their potential influence, to experimentally reduce their magnitude as far as possible, all this requires many years of experience which, indeed, constitutes the ultimate art of measurement.

Nevertheless, the mathematical procedures providing the boundaries for the confining error intervals are not necessarily complicated. All sources which are to be considered should be listed and investigated with respect to the

kind of influence they exert. Some of them will act directly, others within functional relationships. Then, the overall effect to be anticipated should be estimated on the basis of a worst-case reckoning.

In the following we will show that it is always feasible to confine f through an interval symmetrical to zero: if there are experimental findings definitely speaking against such an interval, we should use this information and subtract the term

$$\frac{(f_1 + f_2)}{2}$$

from both the asymmetrical boundaries and the measured data. Thus, we arrive at an interval of the form

$$-f_s \leq f \leq f_s\,; \quad f_s = \frac{(f_2 - f_1)}{2}\,, \tag{2.2}$$

and a new set of data $x'_l = x_l - (f_1 + f_2)/2$, $l = 1, \ldots, n$, where, for convenience, we should abstain from explicitly priming the data. Rather, we should tacitly assume that the corrections have already been made.

Thus, our error model assumes normally distributed random errors and unknown systematic errors of property (2.2). The latter are understood to bias the measuring process. We observe:

The basic error equation of measurement for non-drifting measuring devices (operating in a state of statistical control) is given by

$$x_l = x_0 + \varepsilon_l + f\,; \quad l = 1, \ldots, n \qquad -f_s \leq f \leq f_s\,. \tag{2.3}$$

While the random errors ε_l are assumed to be normally distributed, the unknown systematic error f is considered a time-constant perturbation.

There may be situations in which the effects of perturbations are known to one group of persons but not to another. Then, the first group might wish to speak of systematic deviations while the second group has no other choice than to continue to refer to systematic errors. Should such a distinction turn out to be relevant, it is proposed agreeing on the definition that

- a systematic deviation denotes a time-constant quantity identified in magnitude and sign, while
- an unknown systematic error designates a time-constant quantity unidentified in magnitude and sign.

In the following, we shall exclusively address the latter, i.e. unknown systematic errors, and to be brief, we shall simply call them systematic errors, as by their very nature, errors are always unknown.

Finally, Fig. 2.2 particularizes the measuring process depicted in Sect. 1.1. It may happen that the mathematical representation of the physical model under consideration, for numerical or physical reasons, calls for approximations. Even hypotheses may enter, e.g. when a physical model is to be tested

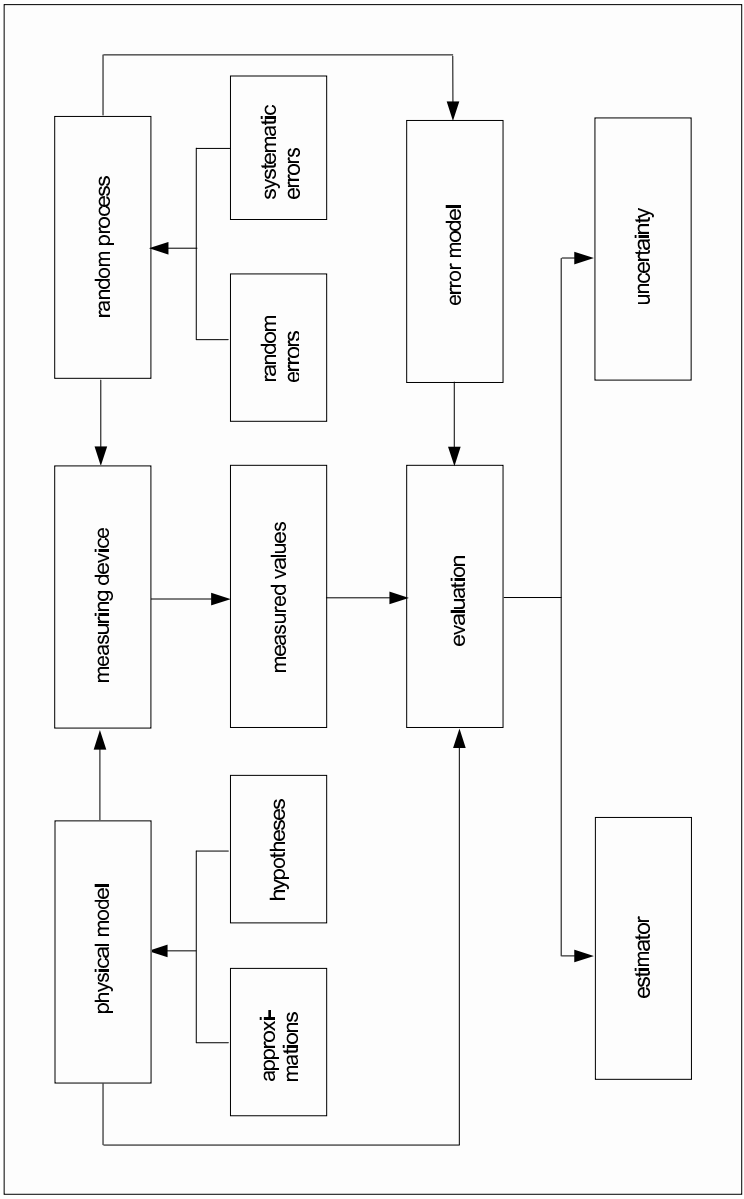


Fig. 2.2. Diagrammed measuring process

by experiment. The design of the measuring device complies with the mathematical formulation of the physical model.

Let us now discuss the still controversial question of whether or not systematic errors should be randomize by means of postulated probability den-

sities. We are sure the experimenter has no chance of influencing the actual values of systematic errors entering his measurements. Doubtless, in that he is confronted with fortuitous events. On the other hand, the decisive question seems to be whether or not he is in a position to alter those systematic errors. In general, the answer will be negative.

Disregarding the efforts to be made, the experimenter could think of disassembling and reassembling the measuring device many a time hoping to vary its systematic errors. Yet, he might not be in a position to do that either for fear of damaging or even destroying some of the components or on account of principle reasons.

Furthermore, the experimenter could try to vary the environmental conditions. This, however, might be difficult to achieve, and if he could do this, on account of the complexity of the interactions the new state might offer no more information than the previous one.

After all, even if the experimenter had the intention to vary his systematic errors, the prospects of success will be limited so that a complete repetition of the measurements under "new conditions" need not necessarily be helpful.

Instead, we ask what properties a formalism, which abstains from assigning probability densities to systematic errors, should have. From the outset it is clear that such an approach will be incompatible with the essential features of the classical Gaussian formalism, thus making it necessary to start the revision from scratch. This might be seen a disadvantage. On the other hand, the time-constancy of unknown systematic errors doubtlessly manifests physical reality, while feeding randomized unknown systematic errors into the classical Gaussian formalism produces quite a series of formal as well as experimental contradictions.

In statistical terms, estimators affected by unknown systematic errors are biased. At the same time, postulated densities would formally cancel biases thus contradicting reality.

As has been mentioned the treatment of several random variables asks for so-called covariances. The nature of the latter is either theoretical or empirical, depending on whether the covariances are taken from parent distribution or from samples of finite size. Obviously, randomized unknown systematic errors only possess theoretical expectations while physical experiments, on the other hand, will never produce expectations but just estimators. Now, even if stationary measuring processes will certainly not exhibit couplings between random and unknown systematic errors, as long as the latter are treated probabilistically, on account of purely formal reasons we are entitled to ask for covariances between the randomized and the truly random errors. – Up to now, a convincing answer to the question of how this might be accomplished does not seem to be at hand.

The analysis of variance attempts to find out whether or not different sets of empirical data of varying origins relating to one and the same physical quantity might have suffered from systematic effects. However, as we

presently know, empirical data sequences are almost surely charged with systematic errors so that any effort to refer to classical test criteria would be superfluous from the outset. In particular, there seems to be no chance to try to generalize the analysis of variance to include unknown systematic errors by means of postulated densities, Sect. 4.3.

In least squares adjustments, the minimized (and appropriately weighted) sum of squared residuals should approximate the number of degrees of freedom of the linear system. However, as empirical observations repeatedly show, this relationship scarcely applies. Rather, as a rule, the aforesaid sum exceeds the number of degrees of freedom appreciably and it suggests attributing this discrepancy to randomized systematic errors, i.e. though the latter have been randomized by postulated densities, the experiment invariably keeps them constant thus revealing the untenability of the randomization concept.

Disregarding all conflicting points, i.e. when systematic errors are randomized, one could, nevertheless, set about defining uncertainty intervals. However, the associated formalism necessarily brings about the geometrical combination of random and systematic errors and thus bans clear and concise decisions. In particular, the experimenter would stay in doubt whether or not his uncertainty localized the true value of his measurand. This, unfortunately, implies the failure of traceability within the system of physical quantities and so disentitles metrology of its objectivity.

Ostensibly, postulated densities for systematic errors would save the Gaussian error calculus. At the same time, this procedure abolishes the consistency between mathematics and physics.

The only way out seems to be to revise the Gaussian formalism from scratch. That Gauß[1] himself strictly refused to include systematic errors in his considerations should be understood as a clear warning sign – otherwise, as he knew, his formalism would not have been operative.

Indeed, the situation becomes different when systematic errors enter in the form of time-constant perturbations. Then, as explained above, random and systematic errors remain strictly separated and combine arithmetically. Also, when properly done, this approach allows the influence of random errors to be treated by means of Student's statistics and the influence of systematic errors by worst case estimations. The associated formalism is clear and concise. In particular, so-defined measurement uncertainties localize the true values of the measurands "quasi-safely" thus ensuring traceability from the start.

However, the announced reference to Student's statistics calls for a paradigm shift inasmuch as we shall have to introduce what might be called well-defined measuring conditions. These ask for equal numbers of repeated measurements for each of the variables entering the error propagation. For apparent reasons, well-defined measuring conditions allow the complete em-

[1]Though this is the proper spelling, in what follows, we shall defer to the more common notation Gauss.

pirical variance–covariance matrices of the input data to be established and, as will become visible, just these matrices lead us back to Student's statistics.

Nonetheless, to require equal numbers of repeat measurements conflicts with common practice. Possibly, unequal numbers of repeat measurements reflect the historical state of communication which, in the past, experimenters and working groups had to cope with. In other words, they virtually had no other choice. However, in the age of desk computers and the Internet, working groups can easily agree on common numbers of repeat measurements, and, by the same token, they can exchange their raw data.

In the end it seems to be more advantageous to forego excessive numbers than to apply questionable, at least clumsy procedures of data evaluation. Firstly, any physical result may not significantly depend on the numbers of repeat measurements and, secondly, questionable uncertainties will tend to blur the primary goal of safely localizing the true values of the measurands.

In view of the high costs Big Physics involves, we should not hesitate to call for well-defined measuring conditions, all the more the experimental efforts remain limited while the attainable benefits promise to be considerable.

2.2 Random Variables, Probability Densities and Parent Distributions

It seems appropriate to formalize the functioning of measuring devices by means of random variables. From a pragmatic point of view, on the one hand we have

- the set of all measured values which the measuring instruments can produce, and on the other hand
- the mathematically abstract definition of random processes and random variables which imply that any number generated by a random process may be understood as the realization of a random variable.

Matching the two means assuming that any measured value is a realization of a random variable and any realization of a random variable a measured value.

Let X denote a random variable and let us attempt to identify its realizations $x_1, x_2, \ldots, x_n$ with the measured data. Conceptually, we might expect the experimental set-up to produce an infinite number of different values. However, as the instrument's resolution is finite, we must be content with a random variable the realizations of which are discrete numbers with relatively few decimal places. In particular, we will in no way encounter an infinite number of numerically different readings. Nevertheless, for simplicity and in a formal sense, we shall stick to the notion of continuous random variables assuming that their realizations map the measuring process.

The error model proposed requires that there be but one systematic error f_x superposed on each of the realizations x_l; $l = 1, \ldots, n$. As a result, the

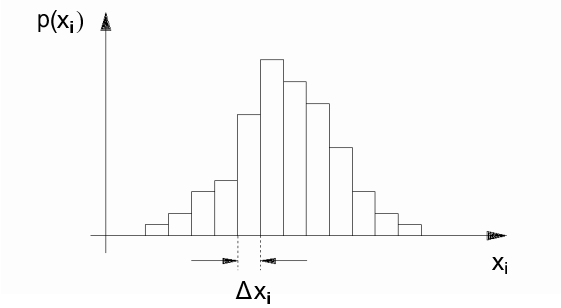


Fig. 2.3. One-dimensional empirical distribution density

actual (unknown) value of the systematic error defines the "center of gravity" of the statistical scattering of the random errors.

When formalizing random errors by means of distribution densities, we shall have to distinguish between theoretical and empirical densities. From the features of empirical densities we may infer the structure of the underlying theoretical densities. To find the empirical distribution density of a sequence of measured data, we assign the data to the horizontal axis and the frequencies of their occurrences to the vertical axis of a rectangular coordinate system. Then, we decompose the horizontal axis into an adequate number r of intervals or "classes" of width Δx_i; $i = 1 \ldots, r$. For any given i, we count the numbers Δn_i of measured values falling within the respective intervals

$$x_i, \ldots, x_i + \Delta x_i\,; \quad i = 1, \ldots, r\,.$$

The empirical distribution density is defined by

$$p(x_i) = \frac{\Delta n_i}{n \Delta x_i}\,; \quad i = 1, \ldots, r\,. \tag{2.4}$$

Here, n denotes the total number of measured data. Obviously, r should have a value which is neither too large nor too small. In the first case, the numbers $p(x_i)$; $i = 1, \ldots, r$ would fluctuate unreasonably strongly, and in the second, they would bring about too coarse a resolution. The $p(x_i)$; $i = 1, \ldots, r$ define a sequence of rectangular columns, Fig. 2.3. The quotient $\Delta n_i / n$ is called the frequency ratio. After all, the shape of an empirical probability density depends not only on the properties of the underlying random process but also on the width of the intervals Δx_i and the number n of data entering the sorting procedure.

From a statistical point of view, the set of measured values x_l; $l = 1, \ldots, n$ defines a sample of size n. Increasing n to any size suggests postulating a so-called parent distribution, encompassing an infinite number of data. Certainly, from an experimental point of view, this is a fiction. Nevertheless, a

parent distribution proves a useful abstraction. In particular, it allows for a probability density, called theoretical or exact, the shape of which is unique.

The theoretical density of the random variable X will be denoted as $p_X(x)$; the symbols x and X express that x is considered to be any realization of the random variable X.

In general, metrology addresses several series of measurements, e.g.

$$x_1, x_2, \ldots, x_n\,; \quad y_1, y_2, \ldots, y_n\,; \quad z_1, z_2, \ldots, z_n \tag{2.5}$$

stemming from different measuring devices. To each of the sequences we assign a random variable, say $X, Y, Z, \ldots$. Clearly, their joint distribution density is multidimensional. Given, there are two random variables, the implied two-dimensional density is constructed as follows: We cover the x, y-plane with a line screen, exhibiting increments Δx_i and Δy_j. Then, we count the numbers Δn_{ij} of pairs x_i, y_j falling within rectangles

$$x_i\,, \ldots,\, x_i + \Delta x_i\,; \quad y_j\,, \ldots,\, y_j + \Delta y_j\,; \quad i, j = 1\,, \ldots,\, r\,.$$

The numbers Δn_{ij} provide the two-dimensional empirical density via

$$p(x_i, y_j) = \frac{\Delta n_{ij}}{n \Delta x_i \Delta y_j}\,; \quad i, j = 1\,, \ldots,\, r\,. \tag{2.6}$$

Figure 2.4 depicts the basic idea. So-called covariances will assist us to allow for dependencies between the series of the data (2.5); they will be discussed in a later section.

Let us revert to (2.4). Another term for frequency ratio, $\Delta n_i/n$, is empirical probability. Obviously

$$\Delta P_i = \frac{\Delta n_i}{n} = p(x_i)\Delta x_i \tag{2.7}$$

denotes the empirical probability of finding Δn_i out of n measured values in an interval ranging from x_i to $x_i + \Delta x_i$. Accordingly, statement (2.6) yields

$$\Delta P_{ij} = \frac{\Delta n_{ij}}{n} = p(x_i, y_j)\Delta x_i \Delta y_j\,, \tag{2.8}$$

denoting the empirical probability of finding Δn_{ij} measured values out of n in a rectangle $x_i, \ldots, x_i + \Delta x_i; y_j, \ldots, y_j + \Delta y_j$. We confine ourselves to this rather technical definition of probability, which relies on the repeatability of physical experiments.

For larger intervals and rectangles, (2.7) and (2.8) turn into sums and double sums respectively. If, instead, we refer to theoretical or exact distribution densities and integral formulations

$$P\{a < X \leq b\} = \int_a^b p_X(x)\mathrm{d}x \tag{2.9}$$

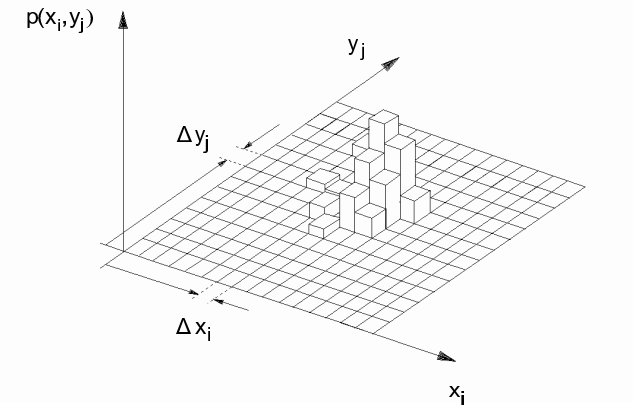


Fig. 2.4. Two-dimensional empirical density

denotes the probability of finding any realization of the random variable X within an interval $a, \ldots, b$ and

$$P\{a < X \leq b\,,\, c < X \leq d\} = \int_a^b \int_c^d p_{XY}(x,y)\mathrm{d}x\mathrm{d}y \tag{2.10}$$

the probability of finding any realizations of the random variables X, Y within a rectangle $a, \ldots, b$; $c, \ldots, d$. Chapter 3 summarizes the distribution densities which will be of relevance here. Subject to their structure, they refer either to one or to more than one normal parent distribution.

As to the interplay between random errors and unknown systematic errors, for stationary measuring processes we shall assume throughout that there are no dependencies or couplings of any kind.

2.3 Elements of Evaluation

In order to find suitable estimators, measured data x_l; $l = 1, \ldots, n$ are usually subjected to arithmetic averaging. In view of the influence of unknown systematic errors, the arithmetic mean

$$\bar{x} = \frac{1}{n}\sum_{l=1}^{n} x_l \tag{2.11}$$

can, however, only be a biased estimator of the true value x_0 of the measurand. As has repeatedly been stated, even if we know that $\bar{x}$ carries a systematic error, we are not in a position to appropriately correct $\bar{x}$. Indeed, all we can do is to design a meaningful measurement uncertainty. According to (2.3), each measured value x_l may formally be written as

$$x_l = x_0 + \varepsilon_l + f\,; \quad l = 1, \ldots, n\,. \tag{2.12}$$

Insertion into (2.11) yields

$$\bar{x} = x_0 + \frac{1}{n}\sum_{l=1}^{n} \varepsilon_l + f\,. \tag{2.13}$$

Even if we assume an arbitrary number of repeat measurements and consider the sum over the random errors to become negligibly small, the arithmetic mean still differs by the actual (unknown) value of the systematic error f from the true value x_0 of the measurand. Hence, $\bar{x}$ is biased with respect to the true value x_0.

Averaging notionally over the infinitely many data $x_l; l = 1, 2, \ldots$ of a normal parent distribution, loosely formulated, the arithmetic mean $\bar{x}$ changes into a parameter

$$\mu = x_0 + f\,, \tag{2.14}$$

where the symmetry of the implied distribution cancels the sum over the random errors. The parameter μ has the property of what will be called an expected value. To be realistic, so-defined quantities remain fictitious, experimentally inaccessible parameters. Inserting (2.14) in (2.13) yields

$$\bar{x} = \mu + \frac{1}{n}\sum_{l=1}^{n} \varepsilon_l\,, \tag{2.15}$$

which reveals that though the average $\bar{x}$ is biased with respect to the true value x_0 of the measurand, it is unbiased with respect to its expectation μ.

Remarkably enough, C. Eisenhart [9] clarified these ostensibly plain relationships in the early 1960s. To the author's knowledge, earlier attempts to clear up the foundations of the Gaussian error calculus have not been made.

To better visualize the relationship between the true value x_0 of the measurand, the expected value μ of the arithmetic mean $\bar{x}$ and the systematic error f we introduce the empirical variance

$$s^2 = \frac{1}{n-1}\sum_{l=1}^{n}(x_l - \bar{x})^2\,, \tag{2.16}$$

which, obviously, measures the scattering of the random errors, Fig. 2.5.

From (2.12) and (2.13) we take that the difference $x_l - \bar{x}$ has cancelled the systematic error f. In (2.16) we could have inserted a factor $1/n$ instead of $1/(n-1)$. However, a so-defined empirical variance would be biased, Sect. 4.2. Let σ^2 denote the expected value of the empirical variance s^2, and, further, s the empirical and σ the theoretical standard deviation. Again, σ^2 is an abstract definition remaining experimentally inaccessible. Nevertheless, in a formal sense, the theoretical variance and the theoretical standard deviation will prove useful many a time.

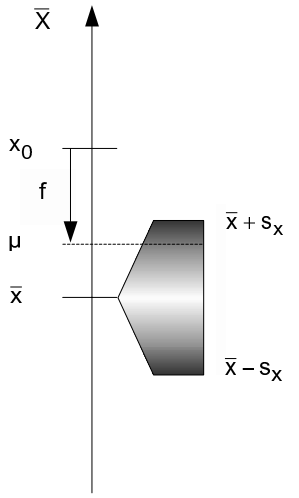


Fig. 2.5. True value x_0, expected value μ, arithmetic mean $\bar{x}$, systematic error f and empirical standard deviation s

The uncertainty of the arithmetic mean should account for the random fluctuations of the x_l as well as for the systematic error f, the latter being bounded by an interval of the form (2.2). As we ask for safe uncertainties, we shall bring the boundaries $\pm f_s$ of that interval to bear. This, in fact, means nothing other than to resort to a worst case estimation.

Equation (2.12) suggests to combine random and systematic errors arithmetically. Hence $u = s + f_s$ appears to be a first reasonable assessment of the uncertainty of the arithmetic mean. For completeness, let us provide the uncertainty, empirical standard deviation and the worst case estimate of the unknown systematic error with indices, then

$$u_{\bar{x}} = s_x + f_{s,x} \,. \tag{2.17}$$

Later, we shall refine the momentousness of random errors in modifying the first term s_x by a factor based on sophisticated statistical considerations. In most cases there will be several series of measurements, so that the means $\bar{x}, \bar{y}, \ldots$ have to be inserted into a given function $\phi(x, y, \ldots)$. Thus, we shall have to assess the uncertainty $u_{\bar{\phi}}$ of a given estimator $\phi(\bar{x}, \bar{y}, \ldots)$ and to quote something like

$$\phi(\bar{x}, \bar{y}, \ldots) \pm u_{\bar{\phi}} \,. \tag{2.18}$$

Fortunately, the considerations presented hitherto may be generalized so that, in correspondence to (2.17), we shall arrive at a similar result, namely

$$u_{\phi} = s_{\phi} + f_{s,\phi} \,. \tag{2.19}$$

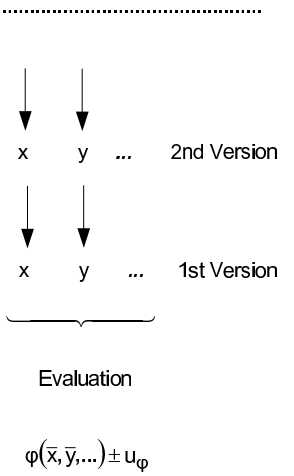


Fig. 2.6. Error propagation, symbolic

The quantities s_ϕ and $f_{s,\phi}$ will be developed in Chap. 6. Also, the first term on the right-hand side may be modified by means of more sophisticated statistical concepts.

In respect of Fig. 2.6, it seems worth adding a remark about the mathematical operations underlying (2.19). The procedures in question will combine n statistically equivalent data sets

$$\begin{array}{l} x_1,\ y_1,\ \ldots \\ x_2,\ y_2,\ \ldots \\ \ldots, \ldots, \ldots \\ x_n,\ y_n,\ \ldots \end{array}$$

where we shall have to brood over the question of how to pair or group the data.

In contrast to the fluctuations of the random errors, the respective systematic errors of the sequences will, of course, not alter, i.e. new information comes in on the part of statistical errors, but not on the part of systematic errors – all we know is that they have assumed (unknown) fixed values within intervals of given lengths.

Apparently, the course of time had shrouded Gauss regular or constant systematic errors with the veil of oblivion. To the author's knowledge, they were rediscovered or possibly even newly discovered by Eisenhart [9] and Wagner [10] inside the national metrology institutes.

Remarkably enough, in certain cases, legal metrology exclusively confines itself to systems of inequalities as given in (2.2), treating and propagating unknown systematic errors in the form of consecutive worst case estimations, thus meeting basic requirements to operate efficiently and safely [26].

3 Densities of Normal Parent Distributions

3.1 One-Dimensional Normal Density

Let the realizations of a random variable X constitute what has been called a parent distribution. If the probability of a realization of X falling within an interval $x, \ldots, x + dx$ is given by

$$p_X(x)dx = \frac{1}{\sigma_x\sqrt{2\pi}} \exp\left(-\frac{x-\mu_x)^2}{2\sigma_x^2}\right) \mathrm{d}x\,, \tag{3.1}$$

the pool of data is said to be normally distributed and $p_X(x)$ itself is called the normal distribution density. While the parameter μ_x marks the center of the density, the parameter σ_x quantifies the broadness of the scattering of the data. To abbreviate, we also say X is $N(\mu_x, \sigma_x)$-distributed.

Figure 3.1 depicts the progression of the density. Following the central limit theorem of statistics, we shall consider the stochastic perturbations of measuring processes to be at least approximately normally distributed – though, of course, there will be exceptions. But even if the statistical behavior of the perturbations is known on that score, metrological applications of (3.1) confront the experimenter with the difficulty, that he is not familiar with the parameters μ_x and σ_x. Though this might be a matter of fact, the author wishes to point to the conflict between theoretically defined parameters of a distribution density and the experimenter's chances of finding appropriate

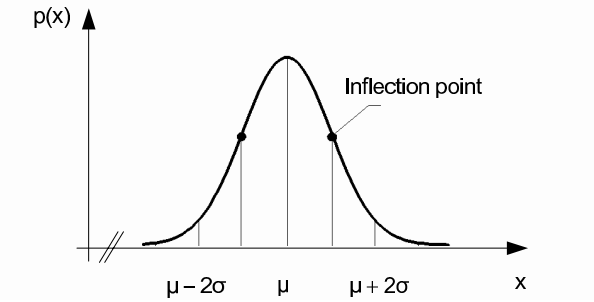


Fig. 3.1. Normal probability density

approximations for them. Strictly speaking, by their very nature, theoretically defined parameters prove to be experimentally inaccessible.

Just to get accustomed to the practical aspect of probability densities, let us try to approximate the numbers Δn_j of the empirical density (2.4) by means of the density $p_X(x)$ implied in (3.1). Assuming normally distributed measured data x_l; $l = 1, \ldots, n$, the number of values falling within any of the r intervals $x_j, \ldots, x_j + \Delta x_j$; $j = 1, \ldots, r$ would be

$$\Delta n_j \approx \frac{n}{\sigma_x \sqrt{2\pi}} \exp\left(-\frac{(x_j - \mu_x)^2}{2\sigma_x^2}\right) \Delta x_j \,. \tag{3.2}$$

Using (3.2), we might wish to design a mean of the data,

$$\bar{x} \approx \sum_{j=1}^{r} x_j \frac{\Delta n_j}{n} \tag{3.3}$$

and also something like a quadratic spread with respect to the so-defined mean,

$$s_x^2 \approx \sum_{j=1}^{r} (x_j - \bar{x})^2 \frac{\Delta n_j}{n} \,. \tag{3.4}$$

However intriguing these attempts may seem, they are meaningless, as they are based upon the unknown parameters μ_x and σ_x.

Let us now refer to the parent distribution and not just to a sample of size n. Then, (3.3) changes into the theoretical mean

$$\mu_x = \int_{-\infty}^{\infty} x \, p_X(x) \mathrm{d}x \tag{3.5}$$

and (3.4) into the theoretical variance

$$\sigma_x^2 = \int_{-\infty}^{\infty} (x - \mu_x)^2 \, p_X(x) \mathrm{d}x \,. \tag{3.6}$$

As is seen, (3.5) and (3.6) simply reproduce the parameters of the density $p_X(x)$. Again, there is no benefit. Nevertheless, the parameters μ_x and σ_x^2, though unknown and inaccessible, are of basic importance as they represent the expectations of the empirical estimators $\bar{x}$ and s_x^2.

In the following, we shall resort to expectations many a time, so that it suggests itself to introduce a convenient symbolism. Instead of (3.5) and (3.6), we shall write

$$\mu_x = E\{X\} \quad \text{and} \quad \sigma_x^2 = E\{(X - \mu_x)^2\}$$

respectively. Here, $E\{\}$ symbolizes the integration while X stands for the integration variable. As has already been done, random variables will be denoted by upper-case letters and their realizations by lower-case letters.[1]

The lesser the scattering of the measured values, the smaller σ_x and the narrower the density $p_X(x)$. Conversely, the wider the scattering, the larger σ_x and the broader the density $p_X(x)$. In particular, given $\mu_x = 0$ and $\sigma_x = 1$, the density (3.1) turns into the so-called standardized normal density $N(0, 1)$. Figure 3.1 underscores the rapid convergence of $p_X(x)$, which gets well along with the experimental behavior of the data – the latter scatter rather to a lesser extent: outside $\mu_x \pm 2\sigma_x$, only relatively few values are to be observed. After all, the tails of the normal density outside, say, $\mu_x \pm 3\sigma_x$, are scarcely significant. The actual situation depends, however, on the intrinsic properties of the particular measuring device.

Nevertheless, confidence intervals and testing of hypotheses just rely upon the tails of distribution densities, which, in pragmatic terms, means that so-defined criteria are based on statistically robust and powerful assertions. After all, the tails of the densities rather play a conceptual role and scarcely appear to be verifiable – at least as long as measuring devices operate in statistically stationary states and do not produce short-time operant systematic errors, so-called outliers, which leave the experimenters in doubt as to whether or not a particular datum might still pertain to one of the tails of the density.

The result of a measurement may not depend significantly on the actual number of repeat measurements, which implies that outliers should not be allowed to play a critical role with regard to the positioning of estimators – though, in individual cases, it might well be recommendable to rely on sophisticated decision criteria. On the other hand, judging from an experimental point of view, it could be more advantageous identifying the causes of outliers.

When we assume that the consecutive numbers $x_1, x_2, \ldots, x_n$ of a sequence of repeat measurements are independent, we impute that the measuring device relaxes before the next measured value is read. Given the measuring device complies with this requirement, we may derive the probability density of the random variable $\bar{X}$ corresponding to the arithmetic mean $\bar{x}$ as follows. To begin with, we generalize our actual notion to consider just one random variable X producing data $x_1, x_2, \ldots, x_n$ and conceive, instead, of an ensemble of statistically equivalent series of measurements. To the first "vertical sequence"

$$x_1^{(1)}, x_1^{(2)}, \ldots, x_1^{(k)}, \ldots$$

of this ensemble

[1] Using Greek letters, however, we shall not explicitly distinguish random variables and their realizations.

$$
\begin{array}{ll}
x_1^{(1)},\, x_2^{(1)},\, x_3^{(1)},\, \ldots,\, x_n^{(1)} & \text{first series} \\
x_1^{(2)},\, x_2^{(2)},\, x_3^{(2)},\, \ldots,\, x_n^{(2)} & \text{second series} \\
\ldots \quad \ldots \quad \ldots \quad \ldots \quad \ldots & \ldots \\
x_1^{(k)},\, x_2^{(k)},\, x_3^{(k)},\, \ldots,\, x_n^{(k)} & \text{k-th series} \\
\ldots \quad \ldots \quad \ldots \quad \ldots \quad \ldots & \ldots
\end{array}
$$

we assign a random variable X_1, to the second a random variable X_2, etc. and, finally, to the n-th a random variable X_n. Then, considering the so-defined variables to be independent and normally distributed, by means of any real constants $b_1, b_2, \ldots, b_n$, we may define a sum

$$Z = b_1 X_1 + b_2 X_2 + \cdots + b_n X_n \,. \tag{3.7}$$

As may be shown [40], see Appendix C, the random variable Z is normally distributed. Putting

$$\mu_i = E\{X_i\} \quad \text{and} \quad \sigma_i^2 = E\{(X_i - \mu_i)^2\}\,; \quad i = 1, ..., n$$

its expectation and scattering are given by

$$\mu_z = \sum_{l=1}^{n} b_l\, \mu_l \quad \text{and} \quad \sigma_z^2 = \sum_{l=1}^{n} b_l^2\, \sigma_l^2 \tag{3.8}$$

respectively. Its distribution density turns out to be

$$p_Z(z) = \frac{1}{\sigma_z \sqrt{2\pi}} \exp\left(-\frac{(z-\mu_z)^2}{2\sigma_z^2}\right) . \tag{3.9}$$

As the X_l; $l = 1, \ldots, n$ are taken from one and the same parent distribution, we have

$$\mu_1 = \mu_2 = \cdots = \mu_n = \mu_x \quad \text{and} \quad \sigma_1^2 = \sigma_2^2 = \cdots = \sigma_n^2 = \sigma_x^2 \,.$$

Hence, setting $b_l = 1/n$; $l = 1, \ldots, n$, the sum Z changes into $\bar{X}$, μ_z into μ_x and, finally, σ_z^2 into σ_x^2/n. Consequently, the probability of finding a realization of $\bar{X}$ within an interval $\bar{x}, \ldots, \bar{x} + \mathrm{d}\bar{x}$ is given by

$$p_{\bar{X}}(\bar{x})\mathrm{d}\bar{x} = \frac{1}{(\sigma_x/\sqrt{n})\sqrt{2\pi}} \exp\left(-\frac{(\bar{x}-\mu_x)^2}{2\sigma_x^2/n}\right) \mathrm{d}\bar{x} \,. \tag{3.10}$$

In the following, we shall refer to the density $p_{\bar{X}}(\bar{x})$ of the arithmetic mean $\bar{X}$ many a time. Error propagation, to be developed in Chap. 6, will be based on linear sums of the kind (3.7), though, admittedly, we shall have to extend the presumption underlying (3.10), as the sum Z turns out to be normally distributed even if the variables X_l; $l = 1, \ldots, n$ prove to be dependent, see

(3.29). Let a final remark be made on the coherence between the level of probability and the range of integration,

$$P = \int_{-a}^{a} p_X(x)\mathrm{d}x\,.$$

Setting $a = 2\sigma_x$, we have

$$0.95 \approx \int_{-2\sigma_x}^{2\sigma_x} p_X(x)\mathrm{d}x\,, \tag{3.11}$$

i.e. $P \approx 95\%$.

3.2 Multidimensional Normal Density

We consider several series of repeat measurements

$$\begin{array}{l} x_1,\, x_2,\, \ldots,\, x_n \\ y_1,\, y_2,\, \ldots,\, y_n \\ \ldots\ \ldots\ \ldots\ \ldots \end{array} \tag{3.12}$$

each comprising the same number n of items. We assign random variables $X, Y, \ldots$ to the series and assume that they refer to different normal parent distributions.

The joint treatment of several series of measurements implies the introduction of covariances. Again, we have to distinguish between empirical and theoretical quantities. While the former pertain to series of measurements of finite lengths, the latter are defined through theoretical distribution densities.

Let us consider just two series of measurements $x_l, y_l, \ldots; l = 1, \ldots, n$. By definition,

$$s_{xy} = \frac{1}{n-1}\sum_{l=1}^{n}(x_l - \bar{x})(y_l - \bar{y}) \tag{3.13}$$

designates the empirical covariance and

$$r_{xy} = \frac{s_{xy}}{s_x s_y}\,; \quad |r_{xy}| \leq 1$$

the empirical correlation coefficient. The quantities s_x and s_y denote the empirical standard deviations, i.e. the square roots of the empirical variances

$$s_x^2 = \frac{1}{n-1}\sum_{l=1}^{n}(x_l - \bar{x})^2 \quad \text{and} \quad s_y^2 = \frac{1}{n-1}\sum_{l=1}^{n}(y_l - \bar{y})^2\,. \tag{3.14}$$

While the expectation of (3.13) leads to the theoretical covariance

$$\sigma_{xy} = E\{S_{xy}\}\,, \tag{3.15}$$

we associate a theoretical correlation coefficient of the form

$$\varrho_{xy} = \frac{\sigma_{xy}}{\sigma_x \sigma_y}\,; \quad |\varrho_{xy}| \leq 1$$

with the empirical quantity r_{xy}. The definitions of σ_{xy} and ϱ_{xy} are formal, as they refer to experimentally inaccessible quantities. It proves convenient to assemble the estimators $s_x^2 \equiv s_{xx}$, $s_{xy} = s_{yx}$, $s_y^2 \equiv s_{yy}$ and the parameters $\sigma_x^2 \equiv \sigma_{xx}$, $\sigma_{xy} = \sigma_{yx}$, $\sigma_y^2 \equiv \sigma_{yy}$ in variance–covariance matrices

$$\boldsymbol{s} = \begin{pmatrix} s_{xx} & s_{xy} \\ s_{yx} & s_{yy} \end{pmatrix} \quad \text{and} \quad \boldsymbol{\sigma} = \begin{pmatrix} \sigma_{xx} & \sigma_{xy} \\ \sigma_{yx} & \sigma_{yy} \end{pmatrix} \tag{3.16}$$

respectively, where it is assumed that they will be non-singular. In this case, they are even positive definite, see Appendix B.

Given that the random variables X and Y are normally distributed, the probability of finding a pair of realizations in any rectangle $x, \ldots, x + \mathrm{d}x$; $y, \ldots, y + \mathrm{d}y$ follows from

$$p_{XY}(x,y)\mathrm{d}x\mathrm{d}y = \frac{1}{2\pi|\boldsymbol{\sigma}|^{1/2}} \exp\Bigg(-\frac{1}{2|\boldsymbol{\sigma}|}\Big[\sigma_y^2(x-\mu_x)^2 \tag{3.17}$$

$$-2\sigma_{xy}(x-\mu_x)(y-\mu_y) + \sigma_x^2(y-\mu_y)^2\Big]\Bigg)\mathrm{d}x\mathrm{d}y\,,$$

where μ_x and μ_y designate the expectations $E\{X\}$ and $E\{Y\}$ respectively, and $|\boldsymbol{\sigma}|$ the determinant of the theoretical variance–covariance matrix $\boldsymbol{\sigma}$. By means of the vectors

$$\boldsymbol{\zeta} = \begin{pmatrix} x \\ y \end{pmatrix} \quad \text{and} \quad \boldsymbol{\mu} = \begin{pmatrix} \mu_x \\ \mu_y \end{pmatrix}\,,$$

the quadratic form of the exponent in (3.17) may be written as

$$\begin{aligned} q &= \frac{1}{|\boldsymbol{\sigma}|}\left[\sigma_y^2(x-\mu_x)^2 - 2\sigma_{xy}(x-\mu_x)(y-\mu_y) + \sigma_x^2(y-\mu_y)^2\right] \\ &= (\boldsymbol{\zeta}-\boldsymbol{\mu})^{\mathrm{T}}\boldsymbol{\sigma}^{-1}(\boldsymbol{\zeta}-\boldsymbol{\mu})\,. \end{aligned}$$

The symbol "T" which is used, where necessary, as a superscript of vectors and matrices denotes transposes. Evidently, the density (3.17) reproduces the theoretical covariance

$$\sigma_{xy} = E\{(X-\mu_x)(Y-\mu_y)\}$$
$$= \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}(x-\mu_x)(y-\mu_y)p_{XY}(x,y)\mathrm{d}x\mathrm{d}y\,. \tag{3.18}$$

The same applies to the parameters σ_x^2 and σ_y^2. If σ_{xy} vanishes, the series of measurements are called uncorrelated. In this situation, the conventional error calculus tacitly ignores empirical covariances. It is interesting to note that, as long as experimenters refer to unequal numbers of repeat measurements, which is common practice, empirical covariances cannot be formalized anyway. We shall resume the question of how to interpret and handle empirical covariances in due course.

Given that the series of measurements (3.12) are independent, the density $p_{XY}(x,y)$ factorizes and σ_{xy} vanishes, which means the two data series are uncorrelated. Conversely, it is easy to give examples proving that uncorrelated series of measurements may well be dependent [43, 50]. However, with respect to normally distributed data series, a vanishing covariance automatically entails the independence of the pertaining random variables.

Considering m random variables $X_1, X_2, \ldots, X_m$, the theoretical variances and covariances are given by

$$\sigma_{ij} = E\{(X_i-\mu_i)(X_j-\mu_j)\}\;;\quad i,j=1\,,\ldots,\,m\,, \tag{3.19}$$

which, again, we assemble in a variance–covariance matrix

$$\boldsymbol{\sigma} = \begin{pmatrix} \sigma_{11} & \sigma_{12} & \ldots & \sigma_{1m} \\ \sigma_{21} & \sigma_{22} & \ldots & \sigma_{2m} \\ \ldots & \ldots & \ldots & \ldots \\ \sigma_{m1} & \sigma_{m2} & \ldots & \sigma_{mm} \end{pmatrix}\;;\quad \sigma_{ii}\equiv\sigma_i^2\,;\quad \sigma_{ij}=\sigma_{ji}\,. \tag{3.20}$$

If $\mathrm{rank}(\boldsymbol{\sigma}) = m$, the latter is positive definite. If $\mathrm{rank}(\boldsymbol{\sigma}) < m$, it is positive semi-definite, see Appendix B.

Now, let $x_1, x_2, \ldots, x_m$ denote any realizations of the random variables $X_1, X_2, \ldots, X_m$ and let $\mu_1, \mu_2, \ldots, \mu_m$ designate the respective expectations. Then, defining the column vectors

$$\boldsymbol{x} = (x_1\ x_2\ \cdots\ x_m)^{\mathrm{T}} \quad \text{and} \quad \boldsymbol{\mu} = (\mu_1\ \mu_2\ \cdots\ \mu_m)^{\mathrm{T}} \tag{3.21}$$

the associated m-dimensional normal probability density is given by

$$p_{\boldsymbol{X}}(\boldsymbol{x}) = \frac{1}{(2\pi)^{m/2}|\boldsymbol{\sigma}|^{1/2}}\,\exp\left(-\frac{1}{2}(\boldsymbol{x}-\boldsymbol{\mu})^{\mathrm{T}}\boldsymbol{\sigma}^{-1}(\boldsymbol{x}-\boldsymbol{\mu})\right)\,, \tag{3.22}$$

where we assume $\mathrm{rank}(\boldsymbol{\sigma}) = m$.

Let us now consider the random variables $\bar{X}$ and $\bar{Y}$. We put down their theoretical variances

$$\sigma_{\bar{x}\bar{x}} \equiv \sigma_{\bar{x}}^2 = \frac{\sigma_x^2}{n} \quad \text{and} \quad \sigma_{\bar{y}\bar{y}} \equiv \sigma_{\bar{y}}^2 = \frac{\sigma_y^2}{n}\,, \tag{3.23}$$

their theoretical covariance

$$\sigma_{\bar{x}\bar{y}} = \frac{\sigma_{xy}}{n} \tag{3.24}$$

and, finally, their theoretical correlation coefficient

$$\varrho_{\bar{x}\bar{y}} = \frac{\sigma_{\bar{x}\bar{y}}}{\sigma_{\bar{x}}\sigma_{\bar{y}}} = \frac{\sigma_{xy}}{\sigma_x\sigma_y} = \varrho_{xy}\,.$$

After all, the joint distribution density is given by

$$p_{\bar{X}\bar{Y}}(\bar{x},\bar{y}) = \frac{1}{2\pi|\bar{\boldsymbol{\sigma}}|^{1/2}} \exp\left(-\frac{1}{2}(\bar{\boldsymbol{\zeta}}-\boldsymbol{\mu})^{\mathrm{T}}\bar{\boldsymbol{\sigma}}^{-1}(\bar{\boldsymbol{\zeta}}-\boldsymbol{\mu})\right)\,, \tag{3.25}$$

where

$$\bar{\boldsymbol{\zeta}} = \begin{pmatrix}\bar{x}\\ \bar{y}\end{pmatrix} \quad \text{and} \quad \bar{\boldsymbol{\sigma}} = \begin{pmatrix}\sigma_{\bar{x}\bar{x}} & \sigma_{\bar{x}\bar{y}}\\ \sigma_{\bar{y}\bar{x}} & \sigma_{\bar{y}\bar{y}}\end{pmatrix}\,.$$

The quadratic form in the exponent of (3.25),

$$\begin{aligned}\bar{q} &= (\bar{\boldsymbol{\zeta}}-\boldsymbol{\mu})^{\mathrm{T}}\bar{\boldsymbol{\sigma}}^{-1}(\bar{\boldsymbol{\zeta}}-\boldsymbol{\mu})\\ &= \frac{1}{|\bar{\boldsymbol{\sigma}}|}\left[\sigma_{\bar{y}\bar{y}}(\bar{x}-\mu_x)^2 - 2\sigma_{\bar{x}\bar{y}}(\bar{x}-\mu_x)(\bar{y}-\mu_y) + \sigma_{\bar{x}\bar{x}}(\bar{y}-\mu_y)^2\right]\\ &= \frac{n}{|\boldsymbol{\sigma}|}\left[\sigma_y^2(\bar{x}-\mu_x)^2 - 2\sigma_{xy}(\bar{x}-\mu_x)(\bar{y}-\mu_y) + \sigma_x^2(\bar{y}-\mu_y)^2\right]\end{aligned} \tag{3.26}$$

defines ellipses $\bar{q} = \text{const}$. Finally, we add the joint density of the variables $\bar{X}_1, \bar{X}_2, \ldots, \bar{X}_m$,

$$p_{\bar{\boldsymbol{X}}}(\bar{\boldsymbol{x}}) = \frac{1}{(2\pi)^{m/2}|\bar{\boldsymbol{\sigma}}|^{1/2}} \exp\left(-\frac{1}{2}(\bar{\boldsymbol{x}}-\boldsymbol{\mu})^{\mathrm{T}}\bar{\boldsymbol{\sigma}}^{-1}(\bar{\boldsymbol{x}}-\boldsymbol{\mu})\right) \tag{3.27}$$

and liken the quadratic forms in the exponents of (3.22) and (3.27),

$$q = (\boldsymbol{x}-\boldsymbol{\mu})^{\mathrm{T}}\boldsymbol{\sigma}^{-1}(\boldsymbol{x}-\boldsymbol{\mu}) \quad \text{and} \quad \bar{q} = (\bar{\boldsymbol{x}}-\boldsymbol{\mu})^{\mathrm{T}}\bar{\boldsymbol{\sigma}}^{-1}(\bar{\boldsymbol{x}}-\boldsymbol{\mu})\,. \tag{3.28}$$

Remarkably enough, both are $\chi^2(m)$ distributed, see Sect. 3.3. From $\bar{q}$ we shall derive the variable of Hotelling's density in due course.

Finally, we generalize (3.7), admitting dependence between the variables. This time, however, we shall consider m random variables instead of n, so that

$$Z = b_1X_1 + b_2X_2 + \cdots + b_mX_m\,. \tag{3.29}$$

Let the X_i come from the density (3.22). Then, as is shown e.g. in [40], see also Appendix C, the variable Z is still normally distributed. Its expectation and its variance are given by

$$\mu_z = E\{Z\} = \sum_{i=1}^{m} b_i\,\mu_i \quad \text{and} \quad \sigma_z^2 = E\{(Z-\mu_z)^2\} = \boldsymbol{b}^{\mathrm{T}}\boldsymbol{\sigma}\boldsymbol{b}\,, \tag{3.30}$$

respectively, where $\boldsymbol{b} = (b_1\ b_2\ \ldots\ b_m)^{\mathrm{T}}$. In (3.11) we realized that an interval of length $4\,\sigma_x$ is related to a probability level of about 95%. Yet, under relatively simple circumstances, the number of variables involved may easily be 20 or even more. Let us set $m = 20$ and ask about the probability of finding realizations $x_1, x_2, \ldots, x_m$ of the random variables $X_1, X_2, \ldots, X_m$ within a hypercube symmetrical about zero and having edges of $4\sigma_x$ side length. For simplicity, we assume the random variables to be independent. This probability is given by

$$P \approx 0.95^{20} \approx 0.36\,. \tag{3.31}$$

Not until we extend the side lengths of the edges of the hypercube up to $6\,\sigma_x$ would we come back to $P \approx 95\%$.

3.3 Chi-Square Density and F Density

The chi-square or χ^2 density covers the statistical properties of a sum of independent, normally distributed, standardized and squared random variables. Let X be normally distributed with $E\{X\} = \mu_x$ and $E\{(X-\mu_x)^2\} = \sigma_x^2$. Then, obviously, the quantity

$$Y = \frac{X-\mu_x}{\sigma_x} \tag{3.32}$$

is normal and standardized, as $E\{Y\} = 0$ and $E\{Y^2\} = 1$. Transferred to n independent random variables $X_1, X_2, \ldots, X_n$, the probability of finding a realization of the sum variable

$$\chi^2(n) = \sum_{l=1}^{n} \left[\frac{X_l-\mu_x}{\sigma_x}\right]^2 \tag{3.33}$$

within any interval $\chi^2, \ldots, \chi^2 + \mathrm{d}\chi^2$ is given by

$$p_{\chi^2}(\chi^2, n)d\chi^2 = \frac{1}{2^{n/2}\Gamma(n/2)}(\chi^2)^{n/2-1}\exp\left(-\frac{\chi^2}{2}\right)\mathrm{d}\chi^2\,; \tag{3.34}$$

$p_{\chi^2}(\chi^2, n)$ is called the χ^2 density. As the parameter μ_x is experimentally inaccessible, (3.33) and (3.34) should be modified. This is, in fact, possible. Substituting $\bar{X}$ for μ_x changes (3.33) into

$$\chi^2(n-1) = \sum_{l=1}^{n} \left[\frac{X_l-\bar{X}}{\sigma_x}\right]^2 = \frac{n-1}{\sigma_x^2}S_x^2 \tag{3.35}$$

and (3.34) into

$$p_{\chi^2}(\chi^2,\nu)\mathrm{d}\chi^2 = \frac{1}{2^{\nu/2}\Gamma(\nu/2)}\,(\chi^2)^{\nu/2-1}\exp\left(-\frac{\chi^2}{2}\right)\mathrm{d}\chi^2\,, \tag{3.36}$$

letting $\nu = n-1$. The number ν specifies the degrees of freedom. The expectation of χ^2 is given by

$$\nu = \int_0^\infty \chi^2\, p_{\chi^2}(\chi^2,\nu)\mathrm{d}\chi^2 \tag{3.37}$$

while for the variance we find

$$2\nu = \int_0^\infty (\chi^2-\nu)^2\, p_{\chi^2}(\chi^2,\nu)\mathrm{d}\chi^2\,. \tag{3.38}$$

The χ^2 density will be used to illustrate the idea of what has called well-defined measuring conditions. To this end, let us consider the random variable defined in (3.29),

$$Z = b_1X_1 + b_2X_2 + \cdots + b_mX_m\,, \tag{3.39}$$

and n of its realizations

$$z^{(l)} = b_1x_1^{(l)} + b_2x_2^{(l)} + \cdots + b_mx_m^{(l)}\,; \quad l = 1,2,\ldots,n\,.$$

The sequence $z^{(l)}$; $l = 1,2,\ldots,n$ leads us to the mean and to the empirical variance,

$$\bar{z} = \frac{1}{n}\sum_{l=1}^{n} z^{(l)} \quad \text{and} \quad s_z^2 = \frac{1}{n-1}\sum_{l=1}^{n}(z^{(l)}-\bar{z})^2 \tag{3.40}$$

respectively. As the $z^{(l)}$ are independent,[2] we are in a position to define

$$\chi^2(n-1) = \frac{(n-1)S_z^2}{\sigma_z^2}\,, \tag{3.41}$$

where $\sigma_z^2 = E\{(Z-\mu_z)^2\}$. If $m = 2$, then, as

$$\bar{z} = b_1\bar{x}_1 + b_2\bar{x}_2 \quad \text{and} \quad z^{(l)} - \bar{z} = b_1(x_1^{(l)}-\bar{x}_1) + b_2(x_2^{(l)}-\bar{x}_2)$$

we have

$$s_z^2 = b_1^2s_1^2 + 2b_1b_2s_{12} + b_2^2s_2^2\,. \tag{3.42}$$

[2]Even if the $X_i; i = 1,\ldots,m$ are dependent, the realizations $z^{(l)}$, $l = 1,\ldots,n$ of the random variable Z are independent. This is obvious, as the realizations $x_i^{(l)}$ of X_i, with i fixed and l running, are independent. The same applies to the realizations of the other variables X_j; $j = 1,\ldots,m$; $j \neq i$.

Obviously, the χ^2 as defined in (3.41) presupposes the same number of repeat measurements and includes the empirical covariance s_{12} – whether or not $\sigma_{12} = 0$ is of no relevance.

In error propagation, we generally consider the link-up of several independent series of measurements. Then, although there are no theoretical covariances, we shall nevertheless consider their empirical counterparts (which, in general, will not be zero). If we did not consider the latter, we would abolish basic statistical relationships, namely the beneficial properties of χ^2 as exemplified through (3.41) and (3.42).

Let us return to the quadratic forms q and $\bar{q}$ quoted in (3.28). Assuming $\mathrm{rank}(\boldsymbol{\sigma}) = m$, the matrix $\boldsymbol{\sigma}$ is positive definite so that a decomposition

$$\boldsymbol{\sigma} = \boldsymbol{c}^{\mathrm{T}}\boldsymbol{c} \tag{3.43}$$

is defined. As $\boldsymbol{\sigma}^{-1} = \boldsymbol{c}^{-1}(\boldsymbol{c}^{\mathrm{T}})^{-1}$, we find

$$q = (\boldsymbol{x} - \boldsymbol{\mu})^{\mathrm{T}}\boldsymbol{c}^{-1}(\boldsymbol{c}^{\mathrm{T}})^{-1}(\boldsymbol{x} - \boldsymbol{\mu}) = \boldsymbol{y}^{\mathrm{T}}\boldsymbol{y} = \sum_{i=1}^{m} y_i^2\,, \tag{3.44}$$

where

$$\boldsymbol{y} = (\boldsymbol{c}^{\mathrm{T}})^{-1}(\boldsymbol{x} - \boldsymbol{\mu}) = (y_1\ y_2\ \cdots\ y_m)^{\mathrm{T}}\,. \tag{3.45}$$

Obviously, the components of the auxiliary vector $\boldsymbol{y}$ are normally distributed. Moreover, because of $E\{\boldsymbol{y}\} = 0$ and $E\{\boldsymbol{y}\,\boldsymbol{y}^{\mathrm{T}}\} = \boldsymbol{I}$, where $\boldsymbol{I}$ denotes an $(m \times m)$ identity matrix, they are standardized and independent, i.e. the quadratic form q is $\chi^2(m)$ distributed. The same applies to the quadratic form $\bar{q}$.

The **F density** considers two normally distributed, independent random variables X_1 and X_2. Let S_1^2 and S_2^2 denote their empirical variances implying n_1 and n_2 repeat measurements respectively. Then, the probability of finding a realization of the random variable

$$F = \frac{S_1^2}{S_2^2} = \frac{\chi^2(\nu_1)/\nu_1}{\chi^2(\nu_2)/\nu_2}\,; \quad \nu_1 = n_1 - 1\,, \quad \nu_2 = n_2 - 1 \tag{3.46}$$

in any interval $f, \ldots, f + \mathrm{d}f$ is given by

$$p_F(f;\nu_1,\nu_2)\mathrm{d}f = \left[\frac{\nu_1}{\nu_2}\right]^{\nu_1/2} \frac{\Gamma[(\nu_1+\nu_2)/2]}{\Gamma(\nu_1/2)\Gamma(\nu_2/2)} \frac{f^{\nu_1/2-1}}{[1+(\nu_1/\nu_2)f]^{(\nu_1+\nu_2)/2}}\,\mathrm{d}f\,. \tag{3.47}$$

Obviously, the symbol f denoting the realizations of the random variable F conflicts with the symbol we have introduced for systematic errors. On the other hand, we shall refer to the F density only once, namely when we convert its quantiles into those of Hotelling's density.

3.4 Student's (Gosset's) Density

The one-dimensional normal density is based on two inaccessible parameters, namely μ_x and σ_x. This inspired W.S. Gosset to derive a new density which better suits experimental purposes [2]. Gosset's variable has the form

$$T = \frac{\bar{X} - \mu_x}{S_x/\sqrt{n}}\,, \tag{3.48}$$

where $\bar{X}$ denotes the arithmetic mean and S_x the empirical standard deviation of n independent, normally distributed repeated measurements,

$$\bar{X} = \frac{1}{n}\sum_{l=1}^{n} X_l \quad \text{and} \quad S_x = \sqrt{\frac{1}{n-1}\sum_{l=1}^{n}(X_l - \bar{X})^2}\,.$$

Besides (3.48), we also consider the variable

$$T' = \frac{X - \mu_x}{S_x}\,. \tag{3.49}$$

Inserting (3.35) in (3.48) and (3.49), we find

$$T = \frac{\dfrac{\bar{X} - \mu_x}{\sigma_x/\sqrt{n}}}{\dfrac{S_x/\sqrt{n}}{\sigma_x/\sqrt{n}}} = \frac{\dfrac{\bar{X} - \mu_x}{\sigma_x/\sqrt{n}}}{\sqrt{\dfrac{\chi^2(n-1)}{n-1}}} \quad \text{and} \quad T' = \frac{\dfrac{X - \mu_x}{\sigma_x}}{\dfrac{S_x}{\sigma_x}} = \frac{\dfrac{X - \mu_x}{\sigma_x}}{\sqrt{\dfrac{\chi^2(n-1)}{n-1}}} \tag{3.50}$$

respectively. The numerators are standardized, normally distributed random variables while the common denominator displays the square root of a χ^2 variable divided by $\nu = n - 1$, the number of degrees of freedom.

The realizations of the variables T and T' lie within $-\infty, \ldots, \infty$. The probability of finding a realization of T in any interval $t, \ldots, t + \mathrm{d}t$ is given by

$$p_T(t;\nu)\,\mathrm{d}t = \frac{\Gamma[(\nu+1)/2]}{\sqrt{\nu\pi}\,\Gamma(\nu/2)}\left(1 + \frac{t^2}{\nu}\right)^{-(\nu+1)/2}\mathrm{d}t\,; \quad \nu = n - 1 \geq 1\,, \tag{3.51}$$

$p_T(t;\nu)$ is called the t-density or Student's density. The latter designation is due to Gosset himself who published his considerations under the pseudonym Student. The density (3.51) also applies to the variable T', see Appendix G.

On the right hand side, we may replace ν by $(n-1)$,

$$= \frac{\Gamma(n/2)}{\sqrt{(n-1)\pi}\,\Gamma[(n-1)/2]}\left(1 + \frac{t^2}{n-1}\right)^{-n/2}\mathrm{d}t\,.$$

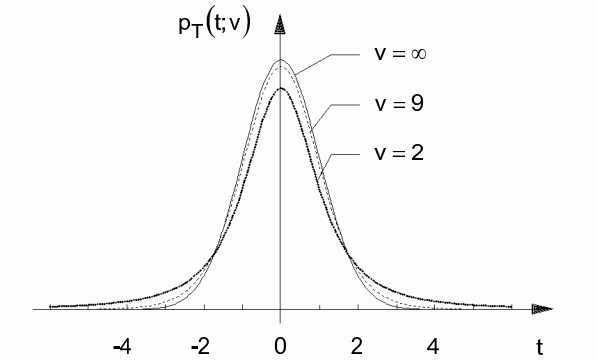


Fig. 3.2. Student's density for $\nu = 2, 9, \infty$

This latter form proves useful when comparing the t-density with its multidimensional analogue, which is Hotelling's density.

Remarkably enough, the number of degrees of freedom, $\nu = n - 1$, is the only parameter of Gosset's density. Its graphic representation is broader but similar to that of the normal density. In particular, it is symmetrical about zero so that the expectation vanishes,

$$E\{T\} = \int_{-\infty}^{\infty} t\, p_T(t;\nu)\, \mathrm{d}t = 0\,. \tag{3.52}$$

For the variance of T we have

$$E\{T^2\} = \int_{-\infty}^{\infty} t^2\, p_T(t;\nu)\, \mathrm{d}t = \frac{\nu}{\nu - 2}\,. \tag{3.53}$$

The larger ν, the narrower the density, but its variance will never fall below 1. Figure 3.2 compares Student's density for some values of ν with the standardized normal density. The the standardized normal density coincides with Student's density as $\nu \to \infty$. Student's density is broader than the standardized normal density, taking into account that the former implies less information than the latter. Moreover, we realize that the greater ν, the smaller the importance of this difference.

The probability of finding any realization of T within an interval of finite length, say, $-t_P\,, \ldots, t_P$ is given by

$$P\{-t_P \le T \le t_P\} = \int_{-t_P}^{t_P} p_T(t;\nu)\, \mathrm{d}t\,. \tag{3.54}$$

Let us once more revert to the meaning of what has been called well-defined measuring conditions. To this end, we consider the random variable

$$Z = b_1 X_1 + b_2 X_2 + \cdots + b_m X_m \,,$$

quoted in (3.39). Assuming that for each of the variables X_i; $E\{X_i\} = \mu_i$; $i = 1, \ldots, m$ there are n repeat measurements, we have

$$\bar{Z} = \frac{1}{n} \sum_{l=1}^{n} Z^{(l)} \,, \quad \mu_z = E\{\bar{Z}\} = \sum_{i=1}^{m} b_i \, \mu_i \,, \quad S_z^2 = \frac{1}{n-1} \sum_{l=1}^{n} (Z^{(l)} - \bar{Z})^2 \,.$$

Now, let us define the variable

$$T(\nu) = \frac{\bar{Z} - \mu_z}{S_z / \sqrt{n}} \,. \tag{3.55}$$

Obviously, the quantity S_z^2 implies the empirical covariances between the m variables X_i; $i = 1, \ldots, m$ be they dependent or not. We have

$$z^{(l)} = b_1 x_1^{(l)} + b_2 x_2^{(l)} + \cdots + b_m x_m^{(l)} \,, \quad \bar{z} = b_1 \bar{x}_1 + b_2 \bar{x}_2 + \cdots + b_m \bar{x}_m$$

so that

$$\begin{aligned} s_z^2 &= \frac{1}{n-1} \sum_{l=1}^{n} \Big[b_1 (x_1^{(l)} - \bar{x}_1) + b_2 (x_2^{(l)} - \bar{x}_2) + \cdots + b_m (x_m^{(l)} - \bar{x}_m) \Big]^2 \\ &= \boldsymbol{b}^{\mathrm{T}} \boldsymbol{s} \, \boldsymbol{b} \,. \end{aligned} \tag{3.56}$$

The matrix notation on the right hand side refers to the empirical variance–covariance matrix $\boldsymbol{s}$ of the input data,

$$\boldsymbol{s} = \begin{pmatrix} s_{11} & s_{12} & \ldots & s_{1m} \\ s_{21} & s_{22} & \ldots & s_{2m} \\ \ldots & \ldots & \ldots & \ldots \\ s_{m1} & s_{m2} & \ldots & s_{mm} \end{pmatrix} \;; \quad s_{ij} = \frac{1}{n-1} \sum_{l=1}^{n} (x_i^{(l)} - \bar{x}_i)(x_j^{(l)} - \bar{x}_j) \tag{3.57}$$

and to an auxiliary vector $\boldsymbol{b}$ of the coefficients b_i; $i = 1, \ldots, m$,

$$\boldsymbol{b} = (b_1 \;\; b_2 \;\; \cdots \;\; b_m)^{\mathrm{T}} \,. \tag{3.58}$$

As mentioned above, empirical covariances are at present treated as if they were bothersome even if the measured data appear in pairs or triples, etc. As long as it is understood that there will be no theoretical covariances, no meaning at all is assigned to their empirical counterparts. Nevertheless, in Sect. 3.3 we have realized that normally distributed measured data are embedded in a coherent complex of statistical statements whose self-consistency should not be called into question. We shall quantitatively deploy these thoughts in the following section.

After all, the question as to whether or not empirical covariances bear information is reduced to the question of whether or not the model of jointly normally distributed measurement data is acknowledged. Here, empirical covariances are considered essential as they preserve the framework of statistics and allow concise and safe statistical inferences.

Examples

Let us ask whether or not the difference between two arithmetic means obtained from different laboratories and relating to one and the same physical quantity might be significant [39] (Vol. II, p. 146, *The problem of two means*).

Let us initially summarize the traditional arguments and refer to different numbers of repeat measurements,

$$\bar{x}_1 = \frac{1}{n}\sum_{l=1}^{n_1} x_1^{(l)}\,; \quad \bar{x}_2 = \frac{1}{n}\sum_{l=1}^{n_2} x_2^{(l)}\,.$$

Then, inevitably, the empirical covariance is to be ignored. After this, we refer to equal numbers of repeat measurements and consider the empirical covariance.

(i) For simplicity, let us disregard systematic errors; consequently we may set $\mu_i = \mu$; $i = 1, 2$. Furthermore, we shall assume equal theoretical variances so that $\sigma_i^2 = \sigma^2$; $i = 1, 2$. Hence, the theoretical variance of the random variable $\bar{Z} = \bar{X}_1 - \bar{X}_2$ is given by

$$\sigma_{\bar{z}}^2 = \frac{\sigma_1^2}{n_1} + \frac{\sigma_2^2}{n_2} = \sigma^2 \frac{n_1 + n_2}{n_1\, n_2}\,.$$

$\bar{Z}$ obviously follows a

$$N\left(0,\ \sigma\sqrt{\frac{n_1 + n_2}{n_1\, n_2}}\right)$$

density. The associated standardized variable is

$$\frac{(\bar{X}_1 - \bar{X}_2)}{\sigma\sqrt{\dfrac{n_1 + n_2}{n_1\, n_2}}}\,.$$

According to (3.50) we tentatively put [38]

$$T = \frac{\dfrac{\bar{X}_1 - \bar{X}_2}{\sigma\sqrt{(n_1 + n_2)/(n_1\, n_2)}}}{\sqrt{\dfrac{\chi^2(\nu^*)}{\nu^*}}} \tag{3.59}$$

attributing degrees of freedom

$$\nu^* = n_1 + n_2 - 2$$

to the sum of the two χ^2-s,

$$\chi^2(\nu^*) = \frac{(n_1 - 1)S_1^2 + (n_2 - 1)S_2^2}{\sigma^2}\,.$$

After all, we consider the random variable

$$T(\nu^*) = \frac{\bar{X}_1 - \bar{X}_2}{\dfrac{\sigma\sqrt{(n_1+n_2)/(n_1\,n_2)}}{\sqrt{\dfrac{(n_1-1)S_1^2+(n_2-1)S_2^2}{\sigma^2}}}}\sqrt{n_1+n_2-2} \tag{3.60}$$

to be t-distributed.

In contrast to this, from (3.55), which is based on $n_1 = n_2 = n$, we simply deduce

$$T(\nu) = \frac{\bar{X}_1 - \bar{X}_2}{\sqrt{S_1^2 - 2S_{12} + S_2^2}}\sqrt{n}\,. \tag{3.61}$$

Clearly, this result is also exact. To compare (3.60) with (3.61), we put $n_1 = n_2$ so that (3.60) changes into

$$T(\nu^*) = \frac{\bar{X}_1 - \bar{X}_2}{\sqrt{S_1^2 + S_2^2}}\sqrt{n}\,. \tag{3.62}$$

While this latter T lacks the empirical covariance S_{12} and refers to degrees of freedom $\nu^* = 2(n-1)$, the T defined in (3.61) relates to degrees of freedom $\nu = (n-1)$, where, of course, we have to consider $t_P(2\nu) < t_P(\nu)$. Remarkably enough, both quantities possess the same statistical properties, namely

$$|\bar{X}_1 - \bar{X}_2| \le t_P(2\nu)\sqrt{S_1^2 + S_2^2}/\sqrt{n}$$

and

$$|\bar{X}_1 - \bar{X}_2| \le t_P(\nu)\sqrt{S_1^2 - 2S_{12} + S_2^2}/\sqrt{n}$$

respectively.

(ii) To be more general, we now admit different expectations, $\mu_1 \neq \mu_2$, and different theoretical variances, $\sigma_1^2 \neq \sigma_2^2$, briefly touching the so-called Fisher–Behrens problem. A solution akin to that presented above does not seem to exist.

Traditionally, the Fisher–Behrens problem refers to $n_1 \neq n_2$. Its implications are extensively discussed in [39] and will therefore not be dealt with here.[3]

B.L. Welch [7] has handled the Fisher–Behrens problem by means of a random variable of the kind

[3] We wish to mention that, from a metrological point of view, the mere notation $\mu_1 \neq \mu_2$ conceals the underlying physical situation. The two means $\bar{x}_1$ and $\bar{x}_2$ may have been determined by means of two different measuring devices, likewise aiming at one and the same physical object, or, alternatively, there might have been two different physical objects and one measuring device or even two different devices.

$$\omega = \frac{(\bar{X}_1 - \bar{X}_2) - (\mu_1 - \mu_2)}{\sqrt{S_1^2/n_1 + S_2^2/n_2}}\,, \quad n_1 \neq n_2\,.$$

This quantity is approximately t-distributed if related to a so-called effective number of degrees of freedom

$$\nu_{\text{eff}} = \frac{(s_1^2/n_1 + s_2^2/n_2)^2}{(s_1^2/n_1)^2/(n_1+1) + (s_2^2/n_2)^2/(n_2+1)} - 2\,,$$

i.e. $\omega(\nu_{\text{eff}})$ leads us back to Student's statistics. Let us recall that both Fisher and Welch considered $n_1 \neq n_2$ a reasonable premise.

Presupposing $n_1 = n_2$, our approach doubtlessly yields an exact

$$T = \frac{(\bar{X}_1 - \bar{X}_2) - (\mu_1 - \mu_2)}{\sqrt{S_1^2 - 2S_{12} + S_2^2}}\sqrt{n}\,. \tag{3.63}$$

After all, when sticking to well-defined measuring conditions bringing the empirical covariance S_{12} to bear the Fisher–Behrens problem is reduced to an ill-defined issue – judged from the kind of statistical reasoning discussed here.

Hotelling [5] has developed a multidimensional generalization of the one-dimensional Student's density. Hotelling's density refers to, say, m arithmetic means each of which implies the same number n of repeat measurements. Again, this latter condition leads us to consider the empirical covariances of the m variables.

Traditionally, Hotelling's variable is designated by T and its realizations, correspondingly, by t. Nevertheless, the respective relationship will disclose by itself whether Student's or Hotelling's variable is meant: the former possesses one, the latter two arguments:

$$\begin{aligned} &t(\nu) && \text{Student's variable}\,,\\ &t(m,n) && \text{Hotelling's variable}\,. \end{aligned}$$

3.5 Fisher's Density

We consider two measurands x and y, assign normally distributed random variables X and Y to them and assume well-defined measuring conditions, i.e. equal numbers of repeat measurements

$$x_1, x_2, \ldots, x_n\,; \quad y_1, y_2, \ldots, y_n\,.$$

Then, Fisher's density specifies the joint statistical behavior of the five random variables

$$\bar{x}, \bar{y}, s_x^2, s_{xy}, s_y^2\,,$$

the two arithmetic means, the two empirical variances and the empirical covariance. Fisher's density implies a metrologically important statement with respect to the empirical covariance of uncorrelated series of measurements. The latter is, as a rule, classified as unimportant if its expectation vanishes. As we shall see, the empirical covariance will nevertheless have a meaning which, ultimately, is rooted in the structure of Fisher's density.

Nonetheless, the present situation is this: Given several measurement results obtained by different laboratories are to be linked with one another, empirical covariances are simply disregarded. On the one hand, this seems to be a matter of habit, on the other hand the original measurement data might not have been preserved and, if, experimenters have carried out different numbers of repeat measurements, which would, a priori rule out the possibility of considering empirical covariances.

In the following we refer to the notation and definitions of Sect. 3.2. Fisher's density

$$p(\bar{x}, \bar{y}, s_x^2, s_{xy}, s_y^2) = p_1(\bar{x}, \bar{y})\, p_2(s_x^2, s_{xy}, s_y^2) \tag{3.64}$$

factorizes into the density p_1 of the two arithmetic means and the density p_2 of the empirical moments of second order. Remarkably enough, the latter,

$$p_2(s_x^2, s_{xy}, s_y^2) = \frac{(n-1)^{n-1}}{4\pi\Gamma(n-2)|\boldsymbol{\sigma}|^{(n-1)/2}} [s_x^2 s_y^2 - s_{xy}^2]^{(n-4)/2} \times \exp\left(-\frac{n-1}{2|\boldsymbol{\sigma}|} h(s_x^2, s_{xy}, s_y^2)\right) ;$$

$$h(s_x^2, s_{xy}, s_y^2) = \sigma_y^2 s_x^2 - 2\sigma_{xy} s_{xy} + \sigma_x^2 s_y^2 , \tag{3.65}$$

does not factorize even if $\sigma_{xy} = 0$. From this we deduce that the model of jointly normally distributed random variables considers the empirical covariance s_{xy} a statistically indispensable quantity. Finally, when propagating random errors taking empirical covariances into account, we shall be placed in a position to define confidence intervals according to Student, irrespective of whether or not the series of measurements are dependent – the formalism (3.55) will always be correct.

In the same way, Hotelling's density, see Sect. 3.6, will provide experimentally meaningful confidence ellipsoids.

In (3.65), we may substitute the empirical correlation coefficient $r_{xy} = s_{xy}/(s_x s_y)$ for the empirical covariance s_{xy} so that

$$p_2(s_x^2, r_{xy}, s_y^2) = \frac{(n-1)^{n-1}}{4\pi\Gamma(n-2)|\boldsymbol{\sigma}|^{(n-1)/2}} s_x^{n-3} s_y^{n-3} [1 - r_{xy}^2]^{(n-4)/2} \times \exp\left(-\frac{n-1}{2|\boldsymbol{\sigma}|} h(s_x^2, r_{xy}, s_y^2)\right) ;$$

$$h(s_x^2, r_{xy}, s_y^2) = \sigma_y^2 s_x^2 - 2\sigma_{xy} r_{xy} s_x s_y + \sigma_x^2 s_y^2 . \tag{3.66}$$

If σ_{xy} vanishes, the empirical correlation coefficient r_{xy} and the two empirical variances s_x^2, s_y^2 obviously turn out to be statistically independent. This situation is, however, quite different from that in which we considered the empirical covariance and the empirical variances. Meanwhile, the error calculus relates to density (3.65) and not to density (3.66). We conclude:

Within the framework of normally distributed data the density of the empirical moments of second order requires us to consider empirical covariances, irrespective of whether or not the data series to be concatenated are dependent.

Apparently, we are now confronted with another problem. Independent series of measurements allow the pairing of the measurement data to be altered. For instance, the sequences $(x_1, y_1); (x_2, y_2); \ldots$ and $(x_1, y_2); (x_2, y_1); \ldots$ would be equally valid. While such permutations in no way affect empirical variances, they do, however, affect the empirical covariance (3.13). In general, each new pairing of data yields a numerically different empirical covariance implying, of course, varying lengths of the pertaining confidence intervals to be deduced from (3.55). This might appear confusing, nevertheless the distribution densities (3.51) and (3.65) willingly accept any such empirical covariance, be it the direct result of measurements or due to permutations in data pairing. In particular, each covariance is equally well covered by the probability statement resulting from (3.51).

On this note, we could even purposefully manipulate the pairing of data in order to arrive at a particular, notably advantageous empirical covariance which, e.g., minimizes the length of a confidence interval.

Should, however, a dependence between the series of measurements exist, the experimentally established pairing of data is to be considered statistically significant and no permutations are admissible, i.e. subsequent permutations abolishing the original pairing are to be considered strictly *improper*.

Wishart generalized Fisher's density to more than two random variables [38]. The considerations presented above apply analogously.

Let us return to the problem of two means, $\bar{X}_1$ and $\bar{X}_2$, see Sect. 3.4. Assuming $\sigma_1^2 = \sigma_2^2 = \sigma^2$ we considered the difference $\bar{Z} = \bar{X}_1 - \bar{X}_2$. Obviously, the variable $\bar{Z}$ relates to a two-dimensional probability density. Even if S_1^2 and S_2^2 refer to independent measurements, the model (3.65) formally asks us to complete the empirical variances through the empirical covariance S_{12} as the empirical moments of second order appear to be statistically dependent. In doing so, statistics tells us that any empirical covariance producible out of the input data is likewise admitted.

3.6 Hotelling's Density

Hotelling's density is the multidimensional analogue of Student's density and presupposes the existence of the density (3.65) of the empirical moments of

second order. To represent Hotelling's density, we refer (3.25). As has been stated, the exponent

$$\begin{aligned}\bar{q} &= (\bar{\boldsymbol{\zeta}} - \boldsymbol{\mu})^{\mathrm{T}} \bar{\boldsymbol{\sigma}}^{-1} (\bar{\boldsymbol{\zeta}} - \boldsymbol{\mu}) \\ &= \frac{1}{|\bar{\boldsymbol{\sigma}}|} \left[\sigma_{\bar{y}\bar{y}} (\bar{x} - \mu_x)^2 - 2\sigma_{\bar{x}\bar{y}} (\bar{x} - \mu_x)(\bar{y} - \mu_y) + \sigma_{\bar{x}\bar{x}} (\bar{y} - \mu_y)^2 \right]\end{aligned} \tag{3.67}$$

is $\chi^2(2)$-distributed. Insertion of

$$\bar{\boldsymbol{\sigma}} = \boldsymbol{\sigma}/n\,, \quad \bar{\boldsymbol{\sigma}}^{-1} = n\boldsymbol{\sigma}^{-1}\,, \quad |\bar{\boldsymbol{\sigma}}| = |\boldsymbol{\sigma}|/n^2 \tag{3.68}$$

has led to

$$\begin{aligned}\bar{q} &= n(\bar{\boldsymbol{\zeta}} - \boldsymbol{\mu})^{\mathrm{T}} \boldsymbol{\sigma}^{-1} (\bar{\boldsymbol{\zeta}} - \boldsymbol{\mu}) \\ &= \frac{n}{|\boldsymbol{\sigma}|} \left[\sigma_{yy} (\bar{x} - \mu_x)^2 - 2\sigma_{xy} (\bar{x} - \mu_x)(\bar{y} - \mu_y) + \sigma_{xx} (\bar{y} - \mu_y)^2 \right] .\end{aligned} \tag{3.69}$$

Hotelling substituted the empirical variance–covariance matrix

$$\boldsymbol{s} = \begin{pmatrix} s_{xx} & s_{xy} \\ s_{yx} & s_{yy} \end{pmatrix} \tag{3.70}$$

for the unknown, inaccessible theoretical variance–covariance matrix $\boldsymbol{\sigma}$ so that $\bar{q}$ formally turned into

$$\begin{aligned}t^2(2,n) &= n(\bar{\boldsymbol{\zeta}} - \boldsymbol{\mu})^{\mathrm{T}} s^{-1} (\bar{\boldsymbol{\zeta}} - \boldsymbol{\mu}) \\ &= \frac{n}{|\boldsymbol{s}|} \left[s_{yy} (\bar{x} - \mu_x)^2 - 2s_{xy} (\bar{x} - \mu_x)(\bar{y} - \mu_y) + s_{xx} (\bar{y} - \mu_y)^2 \right] .\end{aligned} \tag{3.71}$$

Finally, Hotelling confined the s_{xx}, s_{xy}, s_{yy} combinations to the inequality

$$-s_x s_y < s_{xy} < s_x s_y\,; \qquad \left(s_x^2 \equiv s_{xx}\,, \quad s_y^2 \equiv s_{yy}\right)$$

thus rendering the empirical variance–covariance matrix $\boldsymbol{s}$ positive definite. Likewise, $\chi^2(2) = \text{const.}$ and $t^2(2,n) = \text{const.}$ depict ellipses but only the latter, Hotelling's ellipses, are free from unknown theoretical parameters, i.e. they do not rely on the theoretical variances and the theoretical covariance. This is a first remarkable property of Hotelling's density. Another property is that $t^2(2,n)$ equally applies to dependent and independent series of measurements. Consequently, the experimenter may refer to $t^2(2,n)$ without having to know or discover whether or not there are dependencies between the underlying series of measurements. With respect to m measurands, we alter the nomenclature substituting $x_1, x_2, \ldots, x_m$ for x, y so that a vector

$$(\bar{\boldsymbol{x}} - \boldsymbol{\mu}) = (\bar{x}_1 - \mu_1 \; \bar{x}_2 - \mu_2 \; \cdots \; \bar{x}_m - \mu_m)^{\mathrm{T}} \tag{3.72}$$

is obtained in place of $\bar{\boldsymbol{\zeta}} - \boldsymbol{\mu} = (\bar{x} - \mu_x \; \bar{y} - \mu_y)^{\mathrm{T}}$. Thus

$$t^2(m,n) = n(\bar{\boldsymbol{x}} - \boldsymbol{\mu})^{\mathrm{T}} \boldsymbol{s}^{-1} (\bar{\boldsymbol{x}} - \boldsymbol{\mu}) \tag{3.73}$$

is the multidimensional analogue of (3.71), where

$$\begin{gathered} \boldsymbol{s} = \begin{pmatrix} s_{11} & s_{12} & \dots & s_{1m} \\ s_{21} & s_{22} & \dots & s_{2m} \\ \dots & \dots & \dots & \dots \\ s_{m1} & s_{m2} & \dots & s_{mm} \end{pmatrix} ; \\ s_{ij} = \frac{1}{n-1} \sum_{l=1}^{n} (x_{il} - \bar{x}_i)(x_{jl} - \bar{x}_j) ; \quad i,j = 1,\dots,m \end{gathered} \tag{3.74}$$

denotes the empirical variance–covariance matrix of the measured data. Again, we shall assume $\boldsymbol{s}$ to be positive definite [38].

Formally, we again assign random variables $\bar{X}_1, \bar{X}_2, \dots, \bar{X}_m$ to the m means $\bar{x}_1, \bar{x}_2, \dots, \bar{x}_m$. In like manner, we understand the empirical variance–covariance matrix $\boldsymbol{s}$, established through the measurements, to be a particular realization of a random matrix $\boldsymbol{S}$. Hotelling [5] has shown that free from theoretical variances and covariances, a density of the form

$$\begin{gathered} p_T(t;m,n) = \frac{2\Gamma(n/2)}{(n-1)^{m/2}\Gamma[(n-m)/2]\Gamma(m/2)} \frac{t^{m-1}}{[1 + t^2/(n-1)]^{n/2}} ; \\ t > 0 , \quad n > m \end{gathered} \tag{3.75}$$

specifies the probability of finding a realization of the random variable

$$T(m,n) = \sqrt{n(\bar{\boldsymbol{X}} - \boldsymbol{\mu})^{\mathrm{T}} \boldsymbol{S}^{-1} (\bar{\boldsymbol{X}} - \boldsymbol{\mu})} \tag{3.76}$$

in any interval $t, \dots, t + dt$. Accordingly, the probability of the event $T \leq t_P(m,n)$ is given by

$$P\{T \leq t_P(m,n)\} = \int_0^{t_P(m,n)} p_T(t;m,n)\, \mathrm{d}t . \tag{3.77}$$

Figure 3.3 illustrates $p_T(t;m,n)$ for $m = 2$ and $n = 10$. If $m = 1$, (3.75) changes into

$$p_T(t;1,n) = \frac{2\Gamma(n/2)}{(n-1)^{1/2}\Gamma[(n-1)/2]\Gamma(1/2)} \left(1 + \frac{t^2}{n-1}\right)^{-n/2} ,$$

which may be compared with (3.51). Obviously, for $m = 1$, Hotelling's density is symmetric about $t = 0$ and, apart from a factor of 2 in the numerator, identical with Student's density. The latter may be removed by extending the domain of $p_T(t;1,n)$ from $0, \dots, +\infty$ to $-\infty, \dots, +\infty$, which is, however, admissible only if $m = 1$.

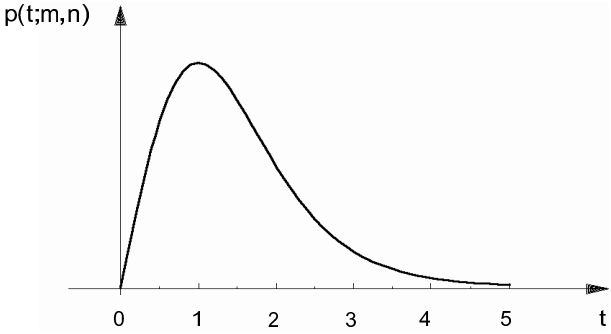


Fig. 3.3. Hotelling's density; $m = 2$; $n = 10$

In order to practically utilize (3.76) and (3.77), we proceed just as we did when discussing Student's density and wished to localize the unknown parameter μ. Following (3.76), we center Hotelling's ellipsoid $t^2(m,n) = \text{const.}$ in $\bar{\boldsymbol{x}}$ and formally substitute an auxiliary vector $\boldsymbol{x}$ for the unknown vector $\boldsymbol{\mu}$. The so-defined confidence ellipsoid

$$t_P^2(m,n) = n(\boldsymbol{x} - \bar{\boldsymbol{x}})^{\mathrm{T}} \boldsymbol{s}^{-1} (\boldsymbol{x} - \bar{\boldsymbol{x}}) \tag{3.78}$$

localizes the point defined by the unknown vector $\boldsymbol{\mu}$ with probability $P\{T \leq t_P(m,n)\}$ as given in (3.77).

This latter interpretation obviously reveals the benefit of our considerations. As is known, the conventional error calculus gets confidence ellipsoids from the exponent of the multidimensional normal probability density and these, unfortunately, imply unknown theoretical variances and covariances. In contrast to this, Hotelling's ellipsoid only needs empirical variances and covariances. Let us again consider the ellipse defined in (3.71). To simplify the notation, we set

$$\alpha = s_{yy}\,, \quad \beta = -s_{xy}\,, \quad \gamma = s_{xx}\,, \quad \delta = \frac{|\boldsymbol{s}|t^2(2,n)}{n}$$

so that

$$\alpha(\bar{x} - \mu_x)^2 + 2\beta(\bar{x} - \mu_x)(\bar{y} - \mu_y) + \gamma(\bar{y} - \mu_y)^2 = \delta\,.$$

From the derivative

$$\bar{y}' = -\frac{\alpha(\bar{x} - \mu_x) + \beta(\bar{y} - \mu_y)}{\beta(\bar{x} - \mu_x) + \gamma(\bar{y} - \mu_y)}$$

we deduce

$$|\bar{x} - \mu_x|_{\max} = \frac{t_P(2,n)}{\sqrt{n}}\sqrt{s_{xx}} \quad \text{and} \quad |\bar{y} - \mu_y|_{\max} = \frac{t_P(2,n)}{\sqrt{n}}\sqrt{s_{yy}}\,.$$

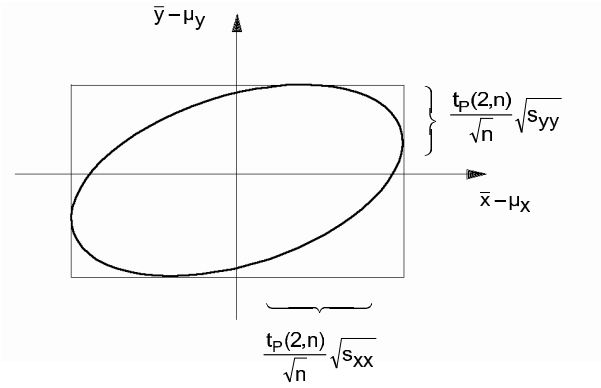


Fig. 3.4. Hotelling's ellipse

Figure 3.4 puts straight that Hotelling's ellipse is included in a rectangle whose side lengths are independent of the empirical covariance s_{xy}. In the case of independent series of measurements, this means: while any permutations within the pairings

$$x_1\,,\,y_1\,;\quad x_2\,,y_2\,;\quad \ldots\,;\quad x_n\,,\,y_n$$

do not affect the empirical variances, the empirical covariance may, however, assume new values, thus rotating Hotelling's ellipse within the aforesaid fixed rectangle. All positions of the ellipse are equally admissible. Up to now, degenerations had been formally excluded. However, admitting them for a moment, we are in a position to state:

The inequality

$$-s_x s_y \le s_{xy} \le s_x s_y$$

(which here includes degenerations) reveals that, given that the two series of measurements are independent, all $(\bar{x}-\mu_x), (\bar{y}-\mu_y)$ *pairs within the rectangle are tolerable.*

This interpretation proves invertible, i.e. in terms of (3.78) we may just as well state: The point (μ_x, μ_y) defining the unknown vector $\boldsymbol{\mu}$ may lie anywhere within a rectangle, centered in $(\bar{x}, \bar{y})$, and having the side lengths

$$2\,\frac{t_P(2,n)}{\sqrt{n}}\sqrt{s_{xx}} \quad \text{and} \quad 2\,\frac{t_P(2,n)}{\sqrt{n}}\sqrt{s_{yy}}$$

respectively. We stress that, given that the series of measurement are dependent, we are not allowed to perform any interchanges within the jointly measured data pairs.

Apparently, a table of quantiles $t_P(m,n)$ of order $P(t_P(m,n))$ according to (3.77) does not exist. Meanwhile, we can use the tabulated quantiles of

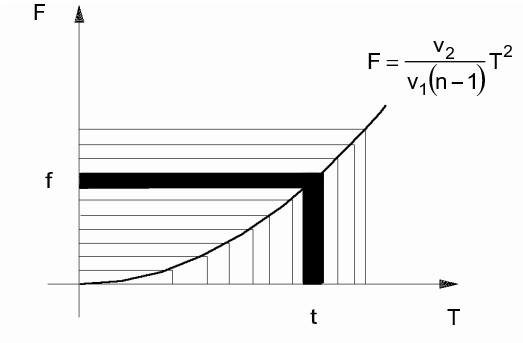


Fig. 3.5. Transformation of Hotelling's density

the F density as there is a relationship between the latter and Hotelling's density.[4]

We ask, given a random variable with probability density F (3.47),

$$p_F(f;\nu_1,\nu_2)\mathrm{d}f = \left[\frac{\nu_1}{\nu_2}\right]^{\nu_1/2} \frac{\Gamma[(\nu_1+\nu_2)/2]}{\Gamma(\nu_1/2)\Gamma(\nu_2/2)} \frac{f^{\nu_1/2-1}}{[1+(\nu_1/\nu_2)f]^{(\nu_1+\nu_2)/2}}\,\mathrm{d}f\,,$$

what is the density $p_T(t)$ of the variable

$$t = \sqrt{\frac{\nu_1}{\nu_2}(n-1)f}\,. \tag{3.79}$$

With a view to Fig. 3.5 we find [43]

$$p_T(t) = p_F\left[\frac{\nu_2}{\nu_1(n-1)}t^2\right]\left|\frac{\mathrm{d}f}{\mathrm{d}t}\right|\,. \tag{3.80}$$

Setting

$$\nu_1 = m\,; \quad \nu_2 = n-m\,; \quad \nu_1+\nu_2 = n \tag{3.81}$$

we easily reconstruct (3.75). Then, from the quantiles of the F density, we infer via

$$P = \int_0^f p_F(f';\nu_1,\nu_2)\,\mathrm{d}f' = \int_0^t p_T(t';m,n)\,\mathrm{d}t' \tag{3.82}$$

the quantiles t of Hotelling's density.

[4] As an exception, here we deviate from the nomenclature agreed on according to which f denotes a systematic error.

Example

Calculate Hotelling's quantile of order P=95%, given $m = 1$ and $n = 11$. As $\nu_1 = 1$ and $\nu_2 = 10$, we have

$$0.95 = \int_0^{f_{0.95}} p_F(f; 1, 10)\, \mathrm{d}f \,.$$

From the table of the F density we infer the quantile $f_{0.95} = 4.96$ so that from (3.79) we obtain Hotelling's quantile $t_{0.95} = 2.2$. As expected, this value indeed agrees with Student's quantile, since $m = 1$.

4 Estimators and Their Expectations

4.1 Statistical Ensembles

Expectations, as theoretical concepts, emerge from integrals and distribution densities. Their experimental counterparts are so-called estimators. The arithmetic mean and the empirical variance

$$\bar{x} = \frac{1}{n}\sum_{l=1}^{n} x_l\,, \quad s_x^2 = \frac{1}{n-1}\sum_{l=1}^{n}(x_l - \bar{x})^2 \tag{4.1}$$

for example, are estimators of the expectations

$$\mu_x = E\{\bar{X}\} = \int_{-\infty}^{\infty} \bar{x}\, p_{\bar{X}}(\bar{x})\mathrm{d}\bar{x} \tag{4.2}$$

and

$$\sigma_x^2 = E\left\{(X-\mu_x)^2\right\} = \int_{-\infty}^{\infty} (x-\mu_x)^2\, p_X(x)\,\mathrm{d}x\,, \tag{4.3}$$

where $p_{\bar{X}}(\bar{x})$ and $p_X(x)$ denote the distribution densities of the random variables $\bar{X}$ and X respectively. While (4.2) is quite obvious, statement (4.3) needs some explanations as the integrand holds a non-linear function of x, namely $\phi(x) = (x-\mu_x)^2$, which is simply averaged by the density $p_X(x)$ of X.

Let X be a random variable with realizations x, and $u = \phi(x)$ a given function. Then, as may be shown, see e.g. [43], the expectation of the random variable $U = \phi(X)$ is given by

$$E\{U\} = \int_{-\infty}^{\infty} u\, p_U(u)\mathrm{d}u = \int_{-\infty}^{\infty} \phi(x)\, p_X(x)\,\mathrm{d}x\,, \tag{4.4}$$

where $p_U(u)$ denotes the density of the variable U and $p_X(x)$ that of the variable X. Analogously, considering functions of several variables, e.g. $V = \phi(X,Y)$, we may set

$$E\{V\} = \int_{-\infty}^{\infty} v\, p_V(v)\, \mathrm{d}v = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \phi(x,y)\, p_{XY}(x,y)\, \mathrm{d}x\, \mathrm{d}y\,. \tag{4.5}$$

Again, $p_V(v)$ constitutes the density of the random variable V and $p_{XY}(x,y)$ the joint density of the random variables X and Y. Thus, (4.4) and (4.5) save us the trouble of developing the densities $p_U(u)$ and $p_V(v)$ when calculating the respective expectations.

In the following, we shall address the expectations of some frequently used empirical estimators. For this, we purposefully rely on a (conceived, fictitious) statistical ensemble of infinitely many identical measuring devices which basically have similar statistical properties and, exactly, one and the same unknown systematic error, Fig. 4.1. From each device, we bring in the same number n of repeat measurements. In a formal sense, the collectivity of the random variables $X^{(k)}$; $k = 1, 2, 3, \ldots$

$$X^{(k)} \Leftrightarrow x_1^{(k)}, x_2^{(k)}, \ldots, x_n^{(k)}\,; \quad k = 1, 2, 3, \ldots \tag{4.6}$$

establishes a statistical ensemble enabling us to calculate expectations.

A measuring device, which is used over a period of many years, may be regarded as approximating an ensemble of the above kind – if only its inherent systematic errors remain constant in time. As has been pointed out, experimenters are pleased to manage with less, namely with systematic errors remaining constant during the time it takes to perform n repeat measurements so that the data remain free from drifts. Moreover, as variations of systematic errors cannot be excluded during prolonged periods of time, their changes should stay within the error bounds conclusively assigned to them from the outset.

Let us conceptualize these ideas. If, as presumed, all measuring devices have the same unknown systematic error $f = \text{const.}$, the data are gathered under conditions of reproducibility. On the other hand, each of the experimental set-ups might also be affected by a specific unknown systematic error. Then the data would be recorded under conditions of comparability. The distinction between reproducibility and comparability induces us to stress once more that reproducibility aims at quite a different thing than accuracy. We shall encounter conditions of comparability in Sect. 12.2 when treating so-called key comparisons.

Obviously, apart from (4.6), the ensemble also implies random variables of the kind X_l; $l = 1, 2, \ldots, n$

$$X_l \Leftrightarrow x_l^{(1)}, x_l^{(2)}, \ldots, x_l^{(k)}, \ldots, \quad l = 1, 2, \ldots, n\,. \tag{4.7}$$

Formally, we now represent the arithmetic mean

$$\bar{x} = \frac{1}{n}(x_1 + x_2 + \cdots + x_n)$$

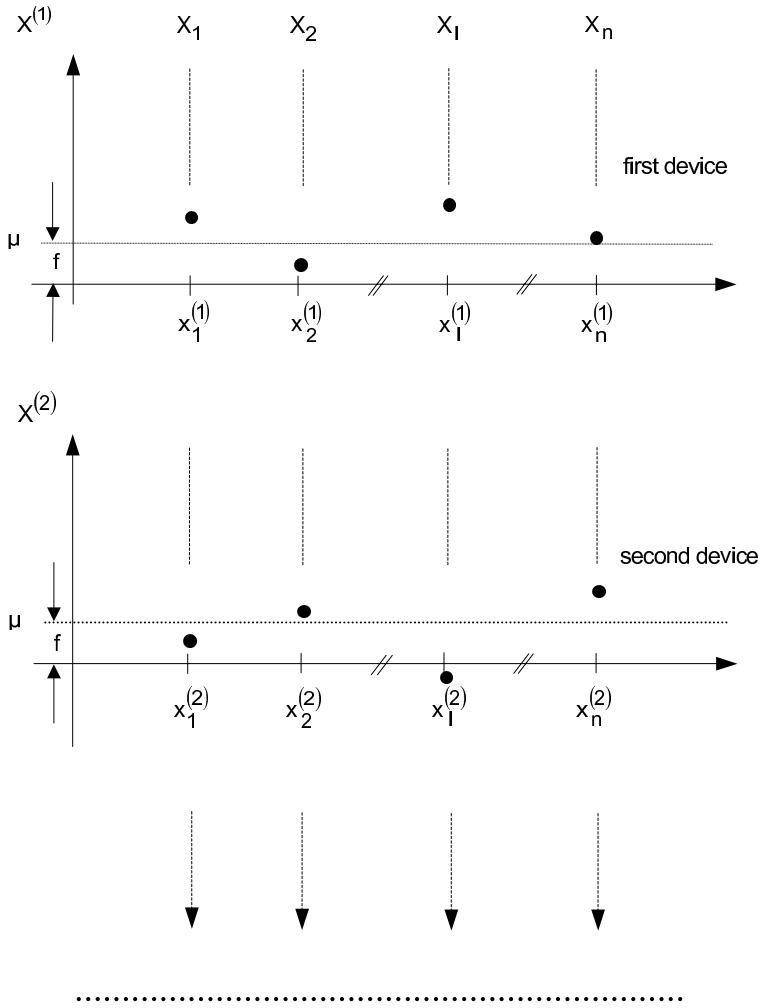


Fig. 4.1. Statistical ensemble of series of repeated measurements, each series comprising n measurements and being affected by one and the same systematic error $f = \text{const}$.

by means of the n realizations of the random variable $X^{(k)}$ as defined in (4.6). For any k we have

$$\bar{x}^{(k)} = \frac{1}{n}\left(x_1^{(k)} + x_2^{(k)} + \cdots + x_n^{(k)}\right) .$$

Certainly, with respect to (4.7), we may just as well introduce the sum variable

$$\bar{X} = \frac{1}{n}(X_1 + X_2 + \cdots + X_n) . \tag{4.8}$$

As assumed, the variables $X_1, X_2, \ldots, X_n$ are independent. We are now in a position to calculate the expectation of the arithmetic mean. Let $p_{\bar{X}}(\bar{x})$ designate the density of the random variable $\bar{X}$ so that

$$E\{\bar{X}\} = \int_{-\infty}^{\infty} \bar{x}\, p_{\bar{X}}(\bar{x})\, \mathrm{d}\bar{x}\,.$$

Referring to (4.5) and (4.8), we find

$$E\{\bar{X}\} = \frac{1}{n} \int_{-\infty}^{\infty} \cdots \int_{-\infty}^{\infty} \times (x_1 + x_2 + \cdots + x_n)\, p_{X_1 X_2 \ldots X_n}(x_1, x_2, \ldots, x_n)\, \mathrm{d}x_1\, \mathrm{d}x_2 \cdots \mathrm{d}x_n\,.$$

In each case, integrating out the "undesired variables" yields 1,

$$E\{\bar{X}\} = \frac{1}{n} \sum_{l=1}^{n} \int_{-\infty}^{\infty} x_l\, p_{X_l}(x_l)\, \mathrm{d}x_l = \mu_x\,. \tag{4.9}$$

After all, the expectation of $\bar{X}$ presents itself as the mean of the expectations of the n random variables $X_1, X_2, \ldots, X_n$, each with the same value μ_x.

4.2 Variances and Covariances

As we recall, the concatenation of the x_l in $\bar{x}$ is linear by definition. The calculation of expectations proves to be more complex if the estimators are of a quadratic nature. Letting μ_x denote the expected value $E\{\bar{X}\}$ of the arithmetic mean $\bar{X}$, we consider the empirical variance as defined through

$$s_x^2 = \frac{1}{n} \sum_{l=1}^{n} (x_l - \mu_x)^2\,. \tag{4.10}$$

Replacing the quantities s_x^2 and x_l with the random variables S_x^2 and X_l respectively, turns (4.10) into

$$S_x^2 = \frac{1}{n} \sum_{l=1}^{n} (X_l - \mu_x)^2\,.$$

The expectation follows from

$$E\{S_x^2\} = \frac{1}{n} E\left\{ \sum_{l=1}^{n} (X_l - \mu_x)^2 \right\} = \frac{1}{n} \sum_{l=1}^{n} E\{(X_l - \mu_x)^2\}\,.$$

But as

$$E\{(X_l - \mu_x)^2\} = \int_{-\infty}^{\infty} (x_l - \mu_x)^2 \, p_{X_l}(x_l) \, \mathrm{d}x = \sigma_x^2 \,,$$

we find

$$E\{S_x^2\} = \sigma_x^2 \,. \tag{4.11}$$

Next we consider the scattering of $\bar{X}$ with respect to μ_x. Each of the devices sketched in Fig. 4.1 produces a specific mean $\bar{x}$. What can we say about the mean-square scattering of $\bar{X}$ relative to the parameter μ_x? We have

$$\begin{aligned} E\{(\bar{X} - \mu_x)^2\} &= E\left\{ \left(\frac{1}{n} \sum_{l=1}^{n} X_l - \mu_x \right)^2 \right\} \\ &= \frac{1}{n^2} E\left\{ \left(\sum_{l=1}^{n} (X_l - \mu_x) \right)^2 \right\} \qquad (4.12) \\ &= \frac{1}{n^2} \Big[E\{(X_1 - \mu_x)^2\} + 2E\{(X_1 - \mu_x)(X_2 - \mu_x)\} \\ &\quad + \cdots + 2E\{(X_{n-1} - \mu_x)(X_n - \mu_x)\} + E\{(X_n - \mu_x)^2\} \Big] \,. \end{aligned}$$

As X_1 and X_2 are independent, the first covariance yields

$$\begin{aligned} E\{(X_1 - \mu_x)(X_2 - \mu_x)\} &= \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} (x_1 - \mu_x)(x_2 - \mu_x) p_{X_1 X_2}(x_1, x_2) \, \mathrm{d}x_1 \, \mathrm{d}x_2 \\ &= \int_{-\infty}^{\infty} (x_1 - \mu_x) p_{X_1}(x_1) \, \mathrm{d}x_1 \int_{-\infty}^{\infty} (x_2 - \mu_x) p_{X_2}(x_2) \, \mathrm{d}x_2 = 0 \end{aligned}$$

and the same applies to the other covariances. As each of the quadratic terms yields σ_x^2 we arrive at

$$E\left\{(\bar{X} - \mu_x)^2\right\} = \frac{\sigma_x^2}{n} \equiv \sigma_{\bar{x}} \,.$$

The empirical variance

$$s_x^2 = \frac{1}{n-1} \sum_{l=1}^{n} (x_l - \bar{x})^2 \tag{4.13}$$

differs from that defined in (4.10) insofar as reference is taken here to $\bar{x}$ and $1/(n-1)$ has been substituted for $1/n$. Rewriting (4.13) in random variables and formalizing the expectation yields

$$E\left\{S_x^2\right\} = \frac{1}{n-1} E\left\{\sum_{l=1}^{n} (X_l - \bar{X})^2\right\} .$$

Due to

$$\begin{aligned}\sum_{l=1}^{n} (X_l - \bar{X})^2 &= \sum_{l=1}^{n} \left[(X_l - \mu_x) - (\bar{X} - \mu_x)\right]^2 \\ &= \sum_{l=1}^{n} (X_l - \mu_x)^2 - 2(\bar{X} - \mu_x) \sum_{l=1}^{n} (X_l - \mu_x) + n(\bar{X} - \mu_x)^2 \\ &= \sum_{l=1}^{n} (X_l - \mu_x)^2 - n(\bar{X} - \mu_x)^2\end{aligned}$$

we get

$$\begin{aligned}E\left\{S_x^2\right\} &= \frac{1}{n-1} E\left\{\sum_{l=1}^{n} (X_l - \mu_x)^2 - n(\bar{X} - \mu_x)^2\right\} \\ &= \frac{1}{n-1}\left(n\sigma_x^2 - n\frac{\sigma_x^2}{n}\right) = \sigma_x^2 .\end{aligned} \tag{4.14}$$

Here again the independence of the measured values x_l; $l = 1, 2, \ldots, n$ proves to be essential. Obviously, estimators (4.10) and (4.13) feature the same expected value but only (4.13) can be realized experimentally.

When calculating $E\{(\bar{X} - \mu_x)^2\}$, we have met the theoretical covariance of the random variables X_1 and X_2. Evidently, this definition applies to any two random variables X and Y with expectations μ_x and μ_y. In general, we have

$$E\{(X - \mu_x)(Y - \mu_y)\} = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} (x - \mu_x)(y - \mu_y)\, p_{XY}(x, y)\, \mathrm{d}x\, \mathrm{d}y = \sigma_{xy} . \tag{4.15}$$

Given X and Y are independent, $p_{XY}(x, y) = p_X(x) p_Y(y)$ and $\sigma_{xy} = 0$.

Before calculating other expectations we extend the conceived statistical ensemble by a second random variable Y, i.e. with each random variable X_l we associate a further random variable Y_l. The consecutive pairs (X_l, Y_l); $l = 1, \ldots, n$ are assumed to be independent, however there may be a correlation between X_l and Y_l. In particular, each X_l is independent of any other $Y_{l'}$; $l \neq l'$.

We now consider the expected value of the empirical covariance

$$s_{xy} = \frac{1}{n} \sum_{l=1}^{n} (x_l - \mu_x)(y_l - \mu_y) . \tag{4.16}$$

Letting S_{xy} denote the associated random variable, we look after the expectation

$$E\{S_{xy}\} = \frac{1}{n} E\left\{ \sum_{l=1}^{n} (X_l - \mu_x)(Y_l - \mu_y) \right\} .$$

Obviously

$$E\{S_{xy}\} = \frac{1}{n} \sum_{l=1}^{n} E\left\{ (X_l - \mu_x)(Y_l - \mu_y) \right\} = \frac{1}{n} n \sigma_{xy} = \sigma_{xy} . \tag{4.17}$$

More effort is needed to cover

$$\begin{aligned} E\left\{ (\bar{X} - \mu_x)(\bar{Y} - \mu_y) \right\} &= \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} (\bar{x} - \mu_x)(\bar{y} - \mu_y)\, p_{\bar{X}\bar{Y}}(\bar{x}, \bar{y})\, \mathrm{d}\bar{x}\, \mathrm{d}\bar{y} \\ &= \sigma_{\bar{x}\bar{y}} . \end{aligned} \tag{4.18}$$

In contrast to (4.15), the expectation (4.18) relates to the less fluctuating quantities $\bar{X}$ and $\bar{Y}$. As

$$\bar{x} - \mu_x = \frac{1}{n} \sum_{l=1}^{n} x_l - \mu_x = \frac{1}{n} \sum_{l=1}^{n} (x_l - \mu_x)$$

$$\bar{y} - \mu_y = \frac{1}{n} \sum_{l=1}^{n} y_l - \mu_y = \frac{1}{n} \sum_{l=1}^{n} (y_l - \mu_y) ,$$

we find

$$\begin{aligned} E\left\{ (\bar{X} - \mu_x)(\bar{Y} - \mu_y) \right\} = \frac{1}{n^2} \int_{-\infty}^{\infty} \cdots \int_{-\infty}^{\infty} \sum_{l=1}^{n} (x_l - \mu_x) \sum_{l'=1}^{n} (y_{l'} - \mu_y) \\ \times p_{X_1 \ldots Y_n}(x_1, \ldots, y_n)\, \mathrm{d}x_1 \ldots \mathrm{d}y_n , \end{aligned}$$

i.e.

$$E\left\{ (\bar{X} - \mu_x)(\bar{Y} - \mu_y) \right\} = \frac{\sigma_{xy}}{n} \equiv \sigma_{\bar{x}\bar{y}} . \tag{4.19}$$

Occasionally, apart from covariances, so-called correlation coefficients are of interest. The latter are defined through

$$\varrho_{xy} = \frac{\sigma_{xy}}{\sigma_x \sigma_y} \quad \text{and} \quad \varrho_{\bar{x}\bar{y}} = \frac{\sigma_{\bar{x}\bar{y}}}{\sigma_{\bar{x}} \sigma_{\bar{y}}} , \quad \text{where} \quad \varrho_{xy} \equiv \varrho_{\bar{x}\bar{y}} . \tag{4.20}$$

The covariances defined in (4.15) and (4.18) rely on experimentally inaccessible parameters. Of practical importance is

$$s_{xy} = \frac{1}{n-1}\sum_{l=1}^{n}(x_l - \bar{x})(y_l - \bar{y})\,. \tag{4.21}$$

As the term within the curled brackets on the right hand side of

$$(n-1)E\{S_{xy}\} = E\left\{\sum_{l=1}^{n}(X_l - \bar{X})(Y_l - \bar{Y})\right\}$$

passes into

$$\begin{aligned}\sum_{l=1}^{n}(X_l - \bar{X})(Y_l - \bar{Y}) &= \sum_{l=1}^{n}\left[(X_l - \mu_x) - (\bar{X} - \mu_x)\right]\left[(Y_l - \mu_y) - (\bar{Y} - \mu_y)\right] \\ &= \sum_{l=1}^{n}(X_l - \mu_x)(Y_l - \mu_y) + n(\bar{X} - \mu_x)(\bar{Y} - \mu_y) \\ &\quad -(\bar{X} - \mu_x)\sum_{l=1}^{n}(Y_l - \mu_y) - (\bar{Y} - \mu_y)\sum_{l=1}^{n}(X_l - \mu_x) \\ &= \sum_{l=1}^{n}(X_l - \mu_x)(Y_l - \mu_y) - n(\bar{X} - \mu_x)(\bar{Y} - \mu_y)\,,\end{aligned}$$

we find

$$(n-1)E\{S_{xy}\} = n\sigma_{xy} - n\frac{\sigma_{xy}}{n} = (n-1)\sigma_{xy}\,,$$

so that

$$E\{S_{xy}\} = \sigma_{xy}\,. \tag{4.22}$$

The empirical covariance (4.21) is unbiased with respect to the theoretical covariance σ_{xy}.

4.3 Elementary Model of Analysis of Variance

The concept of a conceived statistical ensemble helps us to explore the impact of unknown systematic errors on the analysis of variance. As we recall, the latter shall reveal whether or not series of measurements relating to the same physical quantity but carried out at different laboratories are charged by specific, i.e. different unknown systematic errors. But this, quite obviously, conflicts with the approach pursued here. Obviously, given the measured data are biased, the tool *analysis of variance* does no longer appear to be meaningful:

The analysis of variance breaks down, given the empirical data to be investigated are charged or biased by unknown systematic errors.

Let us assume a group of, say m, laboratories has measured one and the same physical quantity, established by one and the same physical object, and that a decision is pending on whether or not the stated results may be considered compatible.

All laboratories have performed the same number n of repeat measurements, so there are means and variances of the form

$$\bar{x}_i = \frac{1}{n}\sum_{l=1}^{n} x_{il}\,; \quad s_i^2 = \frac{1}{n-1}\sum_{l=1}^{n}(x_{il}-\bar{x}_i)^2\,; \quad i = 1,\ldots,m\,. \tag{4.23}$$

We assume the x_{il} to be independent and normally distributed. With regard to the influence of unknown systematic errors, we admit that the expectations μ_i of the arithmetic means $\bar{X}_i$ differ. The expected values of the empirical variances shall, however, be equal

$$E\{\bar{X}_i\} = \mu_i\,, \quad E\{S_i^2\} = \sigma^2\,; \quad i = 1,\ldots,m\,. \tag{4.24}$$

The two error equations

$$\begin{aligned} x_{il} &= x_0 + (x_{il}-\mu_i) + f_i\,, \quad \bar{x}_i = x_0 + (\bar{x}_i - \mu_i) + f_i \\ i &= 1,\ldots,m\,; \qquad l = 1,\ldots,n \end{aligned} \tag{4.25}$$

clearly conflict with the basic idea of analysis of variance. On the other hand, we want to show explicitly why, and how, this classical tool of data analysis breaks down due to the empirical character of the data fed into it.

The analysis of variance defines a grand mean, summing over $N = m \times n$ measuring data x_{il},

$$\bar{x} = \frac{1}{N}\sum_{i=1}^{m}\sum_{l=1}^{n} x_{il} \tag{4.26}$$

and an associated grand empirical variance

$$s^2 = \frac{1}{N-1}\sum_{i=1}^{m}\sum_{l=1}^{n}(x_{il}-\bar{x})^2\,. \tag{4.27}$$

The latter is decomposed by means of the identity

$$x_{il} = \bar{x} + (\bar{x}_i - \bar{x}) + (x_{il} - \bar{x}_i) \tag{4.28}$$

and the error equations (4.25). Thus, (4.27) turns into

$$(N-1)s^2 = n\sum_{i=1}^{m}(\bar{x}_i-\bar{x})^2 + \sum_{i=1}^{m}\sum_{l=1}^{n}(x_{il}-\bar{x}_i)^2 \tag{4.29}$$

as the mixed term vanishes,

$$2\sum_{i=1}^{m}(\bar{x}_i - \bar{x})\sum_{l=1}^{n}(x_{il} - \bar{x}_i) = 0\,.$$

If the systematic errors are zero, the right-hand side of (4.29) would offer the possibility of defining empirical variances s_1^2 and s_2^2, namely

$$(m-1)s_1^2 = n\sum_{i=1}^{m}(\bar{x}_i - \bar{x})^2 \quad \text{and} \quad (N-m)s_2^2 = \sum_{i=1}^{m}\sum_{l=1}^{n}(x_{il} - \bar{x}_i)^2 \tag{4.30}$$

so that

$$(N-1)s^2 = (m-1)s_1^2 + (N-m)s_2^2\,. \tag{4.31}$$

The expectations of both, S_1^2 and S_2^2 should be equal to the theoretical variance σ^2 defined in (4.24), i.e.

$$E\{S_1^2\} = \sigma^2 \quad \text{and} \quad E\{S_2^2\} = \sigma^2\,.$$

Let us first consider the left expectation. As

$$\bar{x}_i = \frac{1}{n}\sum_{l=1}^{n} x_{il} = x_0 + (\bar{x}_i - \mu_i) + f_i\,,$$

and

$$\begin{aligned}\bar{x} = \frac{1}{N}\sum_{i=1}^{m}\sum_{l=1}^{n} x_{il} &= \frac{n}{N}\sum_{i=1}^{m}\left[x_0 + (\bar{x}_i - \mu_i) + f_i\right] \\ &= x_0 + \frac{n}{N}\sum_{i=1}^{m}(\bar{x}_i - \mu_i) + \frac{n}{N}\sum_{i=1}^{m} f_i\,,\end{aligned}$$

we have

$$\bar{x}_i - \bar{x} = \left[(\bar{x}_i - \mu_i) - \frac{n}{N}\sum_{j=1}^{m}(\bar{x}_j - \mu_j)\right] + \left[f_i - \frac{n}{N}\sum_{j=1}^{m} f_j\right]\,,$$

so that

$$E\left\{S_1^2\right\} = \sigma^2 + \frac{n}{(m-1)}\sum_{i=1}^{m}\left[f_i - \frac{n}{N}\sum_{j=1}^{m} f_j\right]^2\,. \tag{4.32}$$

The second expectation follows from

$$\sum_{i=1}^{m}\sum_{l=1}^{n}(x_{il} - \bar{x}_i)^2 = (n-1)\sum_{i=1}^{m} s_i^2\,,$$

so that

$$E\left\{S_2^2\right\} = \sigma^2\,. \tag{4.33}$$

The test ratio of the analysis of variance is the quotient S_1^2/S_2^2, which should be F distributed. On account of (4.32), however, any further consideration appears to be dispensable.

5 Combination of Measurement Errors

5.1 Expectation of the Arithmetic Mean

For convenience's sake, we cast the basic error equation (2.3)

$$x_l = x_0 + \varepsilon_l + f_x\,; \quad l = 1, 2, \ldots, n$$

into the form of an identity

$$x_l = x_0 + (x_l - \mu_x) + f_x\,; \quad l = 1, 2, \ldots, n\,. \tag{5.1}$$

Let us remind that the quantity x_l is a physically measured value while the decomposition (5.1) reflects the error model under discussion. The same applies to the the arithmetic mean

$$\bar{x} = x_0 + (\bar{x} - \mu_x) + f_x \tag{5.2}$$

which, in fact, is a formal representation of

$$\bar{x} = \frac{1}{n}\sum_{l=1}^{n} x_l\,.$$

Let us assign a random variable $\bar{X}$ to $\bar{x}$. Then, obviously, the expectation

$$\mu_x = E\{\bar{X}\} = x_0 + f_x \tag{5.3}$$

puts straight:

The unknown systematic error f_x biases the expectation μ_x of the arithmetic mean $\bar{X}$ with respect to the true value x_0.

In the following we shall design a confidence interval localizing the expectation μ_x of the arithmetic mean. To this end, we refer to the empirical variance

$$s_x^2 = \frac{1}{n-1}\sum_{l=1}^{n}(x_l - \bar{x})^2 \tag{5.4}$$

and to Student's variable

$$T = \frac{\bar{X} - \mu_x}{S_x/\sqrt{n}}\,. \tag{5.5}$$

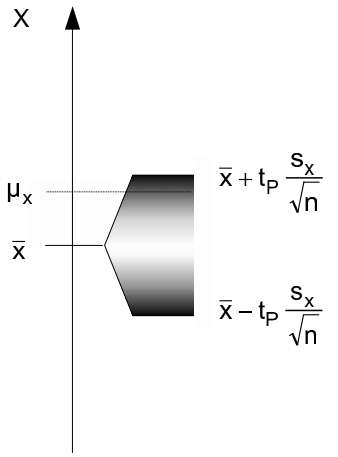


Fig. 5.1. Confidence interval for the expectation μ_x of the arithmetic mean $\bar{X}$

As has been said in (3.54)

$$P\{-t_p \le T \le t_p\} = \int_{-t_p}^{t_P} p_T(t;\nu)\,\mathrm{d}t\,; \quad \nu = n-1 \tag{5.6}$$

specifies the probability of finding any realization t of T in an interval $-t_P, \ldots, t_P$. Often, $P = 0.95$ is chosen. The probability "masses" lying to the left and right of $-t_P$ and t_P respectively, are traditionally denoted as $\alpha/2$. In terms of this partitioning we have $P = 1 - \alpha$.

From (5.5) and (5.6), we infer a statement about the probable location of the random variable $\bar{X}$,

$$P\left\{\mu_x - \frac{t_P(n-1)}{\sqrt{n}}\,S_x \le \bar{X} \le \mu_x + \frac{t_P(n-1)}{\sqrt{n}}\,S_x\right\} = 1-\alpha\,.$$

From the point of view of the experimenter, it will, however, be more interesting to learn about the probable location of the parameter μ_x. Indeed, inverting the above statement yields

$$P\left\{\bar{X} - \frac{t_P(n-1)}{\sqrt{n}}\,S_x \le \mu_x \le \bar{X} + \frac{t_P(n-1)}{\sqrt{n}}\,S_x\right\} = 1-\alpha\,. \tag{5.7}$$

An equivalent statement, which reflects the experimental situation more closely, is obtained as follows: We "draw a sample" $x_1, x_2, \ldots, x_n$ of size n and determine the estimators $\bar{x}$ and s_x^2. Then, as illustrated in Fig. 5.1, we may rewrite (5.7) in the form

$$\bar{x} - \frac{t_P}{\sqrt{n}}\,s_x \le \mu_x \le \bar{x} + \frac{t_P}{\sqrt{n}}\,s_x \quad \text{with probability } P\,. \tag{5.8}$$

This latter statement reveals the usefulness of Student's density: it allows us to localize the unknown parameter μ_x by means of the two estimators $\bar{x}$ and s_x^2. The normal density itself would not admit of such a statement, as the parameter σ_x is inaccessible.

The intervals (5.7) and (5.8) localize the parameter μ_x with probability P as defined in (5.6). The intervals themselves are called confidence intervals and P is called the confidence level.

As has been pointed out, the difference $x_l - \bar{x}$ cancels the systematic error f_x so that the expectation $\sigma_x^2 = E\{S_x^2\}$ of the random variable S_x^2 is unbiased.

Let us keep in mind that the parameter μ_x may differ from the true value x_0 by up to $\pm f_{s,x}$. In order to assess the uncertainty of the mean $\bar{x}$ with respect to the true value x_0, we therefore need to do better.

5.2 Uncertainty of the Arithmetic Mean

The expectation

$$\mu_x = E\{\bar{X}\} = x_0 + f_x\,, \quad -f_{s,x} \le f \le f_{s,x} \tag{5.9}$$

may deviate from x_0 by up to $\pm f_{s,x}$, Fig. 5.2. Hence, as sketched in Fig. 5.3, we define the overall uncertainty $u_{\bar{x}}$ of the estimator $\bar{x}$ as

$$u_{\bar{x}} = \frac{t_P}{\sqrt{n}}\, s_x + f_{s,x}\,. \tag{5.10}$$

The final measurement result reads

$$\bar{x} \pm u_{\bar{x}}\,. \tag{5.11}$$

While (5.8) is a probability statement, (5.11) is not. Instead, we simply argue that this statement localizes the true value x_0 with, say, "factual" or "physical" certainty. Though random errors, emerging from real experiments, may as a rule be considered approximately normally distributed, in general, the extreme tails of the theoretical distribution model $N(\mu_x, \sigma_x)$ seem to be lacking. Relating t_P to, say, $P = 95\%$, this in turn means that we may assume the interval (5.8) to localize μ_x quasi-safely.

The fact that the systematic error f_x enters into (5.11) in the form of a worst case estimate might reflect an overestimation. On the other hand, the experimenter does not have any means at his disposal to shape the uncertainty (5.10) more favorably, i.e. more narrowly. If he nevertheless compressed it, he would run the risk of forgoing the localization of the true value x_0 so that, as a consequence, all his efforts and metrological work would have been futile and, in particular, he might miss metrology's strict demand for traceability.

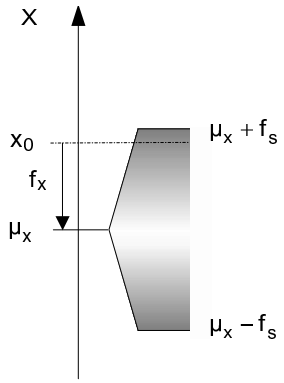


Fig. 5.2. Difference between the expected value μ_x and the true value x_0

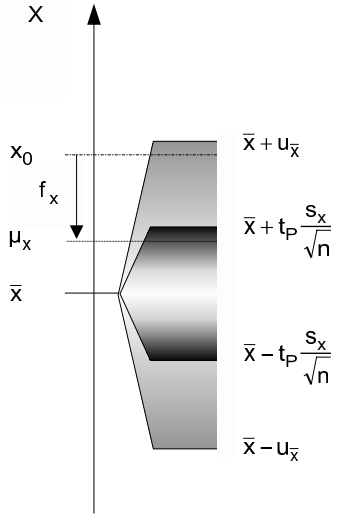


Fig. 5.3. Uncertainty $u_{\bar{x}}$ of the arithmetic mean $\bar{x}$ with respect to the true value x_0

Example

Legal SI-based units are defined verbally – in this respect, they are faultless. Albeit their realizations are blurred as they suffer from experimental imperfections. We consider the base units volt (V), ohm (Ω) and ampere (A). As Fig. 5.4 illustrates, the (present) realization of the SI unit ampere relies on two terms,

$$1\,\mathrm{A} = 1\,\mathrm{A_L} + c\,.$$

Here $1\,\mathrm{A_L}$ designates the laboratory ampere. This should coincide with the theoretically defined SI ampere 1 A. However, as the former deviates from

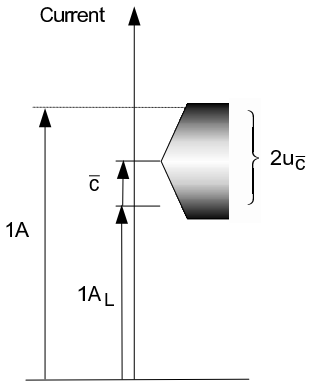


Fig. 5.4. Realization of the SI unit ampere. The quantities 1 A and 1 A_L symbolize the SI ampere and the laboratory ampere respectively

the latter, a correction c needs to be applied. The correction is obtained either from other experiments or from a least squares fit to the fundamental constants of physics. Measured in laboratory units A_L, the correction is given in terms of an average $\bar{c}$ and an uncertainty $u_{\bar{c}}$ so that

$$1\mathrm{A} = 1\mathrm{A_L} + (\bar{c} \pm u_{\bar{c}}) = (1\mathrm{A_L} + \bar{c}) \pm u_{\bar{c}}\,.$$

On the other hand, the distinction between theoretically defined units and their experimentally realized counterparts may also be expressed in the form of quotients. To this end, so-called conversion factors have been introduced. The conversion factor for the ampere is defined by

$$K_\mathrm{A} = \frac{1\mathrm{A_L}}{1\mathrm{A}}\,.$$

Let $\{c\}$ denote the numerical value[1] of c so that $\bar{c} = \{\bar{c}\}\mathrm{A_L}$. Then

$$K_\mathrm{A} = \frac{1}{1 + \{\bar{c}\}} \quad \text{or, equivalently,} \quad \{\bar{c}\} = \frac{1 - K_\mathrm{A}}{K_\mathrm{A}}\,.$$

The uncertainty u_{K_A}, given $u_{\{\bar{c}\}}$, will be derived in Sect. 5.3. Analogous relations refer to the SI units volt and ohm:

$$1\mathrm{V} = 1\mathrm{V_L} + (\bar{a} \pm u_{\bar{a}}) = (1\mathrm{V_L} + \bar{a}) \pm u_{\bar{a}}\,,$$

$$K_\mathrm{V} = \frac{1\mathrm{V_L}}{1\mathrm{V}} = \frac{1}{1 + \{\bar{a}\}}\,, \quad \{\bar{a}\} = \frac{1 - K_\mathrm{V}}{K_\mathrm{V}}\,,$$

$$1\Omega = 1\Omega_\mathrm{L} + (\bar{b} \pm u_{\bar{b}}) = (1\Omega_\mathrm{L} + \bar{b}) \pm u_{\bar{b}}\,,$$

$$K_\Omega = \frac{1\Omega_\mathrm{L}}{1\Omega} = \frac{1}{1 + \{\bar{b}\}}\,, \quad \{\bar{b}\} = \frac{1 - K_\Omega}{K_\Omega}\,.$$

[1] e.g. the unit is suppressed.

For the realization of the units volt and ohm, Josephson's and von Klitzing's quantum effects

$$U_J = \frac{h}{2e}\,\nu \quad \text{and} \quad R_H = \frac{h}{ie^2}\,; \quad i = 1, 2, 3, \ldots$$

respectively, are of tremendous importance; h denotes Planck's constant, e the elementary charge and ν high-frequency radiation ($\approx 70\,\mathrm{GHz}$). Unfortunately, the uncertainties of the leading factors $h/(2e)$ and $R_H = h/e^2$ are still unsatisfactory. Nevertheless, sophisticated predefinitions

$$2e/h = 483\,597.\mathbf{9}\,\mathrm{GHz/V}\ \text{(exact)}\,; \quad h/e^2 = 25.812\,80\mathbf{7}\,\mathrm{K\Omega}\ \text{(exact)}$$

enable experimenters to exploit the remarkable reproducibilities of quantum effects, i.e. to adjust the sums $1\,\mathrm{V_L} + \bar{a}$ and $1\,\Omega_\mathrm{L} + \bar{b}$; the uncertainties $u_{\bar{a}}$ and $u_{\bar{b}}$ remain, however, unaffected.

We finally add the relationships between the constants a, b, c and the conversion coefficients $K_\mathrm{V}, K_\Omega, K_\mathrm{A}$. From

$$1\,\mathrm{V} = 1\,\Omega\ 1\,\mathrm{A} \quad \text{and} \quad 1\,V_\mathrm{L} = 1\,\Omega_\mathrm{L}\,1\,\mathrm{A_L}$$

we find

$$[1 + \{\bar{a}\}]\ \mathrm{V_L} = \left[1 + \{\bar{b}\}\right]\ \Omega_\mathrm{L}\,[1 + \{\bar{c}\}]\ \mathrm{A_L}$$

and, assuming $\{\bar{a}\}, \{\bar{b}\}, \{\bar{c}\} <\approx 10^{-6}$, by approximation

$$\{\bar{a}\} = \{\bar{b}\} + \{\bar{c}\}\,.$$

Similarly, from

$$\frac{\mathrm{V_L}}{K_\mathrm{V}} = \frac{\Omega_\mathrm{L}}{K_\Omega}\,\frac{\mathrm{A_L}}{K_\mathrm{A}}$$

we obtain

$$K_\mathrm{V} = K_\Omega K_\mathrm{A}\,.$$

5.3 Uncertainty of a Function of One Variable

The simplest case of error propagation is the function of one variable, say $\phi(x)$, e.g. $\phi(x) = \ln x$, $\phi(x) = 1/x$, etc. In most cases, error propagation within functional relationships takes place on the basis of *linearized* Taylor series expansions. Whether or not this is admissible depends on the magnitude of the measurement uncertainties of the input data, in this case of the uncertainty $u_{\bar{x}}$ of the quantity $\bar{x}$, and on the analytical behavior of the considered function in the neighborhood of $\bar{x} \pm u_{\bar{x}}$. Assuming $\phi(x)$ to behave linearly enough, the error equations

$$x_l = x_0 + (x_l - \mu_x) + f_x\,, \quad \bar{x} = x_0 + (\bar{x} - \mu_x) + f_x$$

lead us to

$$\phi(x_l) = \phi(x_0) + \frac{\mathrm{d}\phi}{\mathrm{d}x}\Big|_{x=x_0}(x_l - \mu_x) + \frac{\mathrm{d}\phi}{\mathrm{d}x}\Big|_{x=x_0} f_x + \cdots$$

$$\phi(\bar{x}) = \phi(x_0) + \frac{\mathrm{d}\phi}{\mathrm{d}x}\Big|_{x=x_0}(\bar{x} - \mu_x) + \frac{d\phi}{dx}\Big|_{x=x_0} f_x + \cdots \tag{5.12}$$

so that[2]

$$\phi(x_l) - \phi(\bar{x}) = \frac{\mathrm{d}\phi}{\mathrm{d}\bar{x}}(x_l - \bar{x})\,; \quad l = 1, 2, \ldots, n\,. \tag{5.13}$$

Here it is assumed that

- the expansions may be truncated after their linear terms and that
- the derivative in x_0 may be approximated by the derivative in $\bar{x}$.

Furthermore, for the sake of lucidity, an equal sign has been introduced which, actually, is of course incorrect. Finally, we shall assume that

- by approximation, the derivatives may be treated as constants.

Within the framework of these approximations, the expected value of the random variable $\phi(\bar{X})$,

$$\mu_\phi = E\left\{\phi(\bar{X})\right\} = \phi(x_0) + \frac{\mathrm{d}\phi}{\mathrm{d}\bar{x}} f_x\,, \tag{5.14}$$

presents itself as the sum of the true value $\phi(x_0)$ and a *bias* expressing the propagated systematic error

$$f_\phi = \frac{\mathrm{d}\phi}{\mathrm{d}\bar{x}} f_x\,; \quad -f_{s,x} \le f_x \le f_{s,x}\,. \tag{5.15}$$

Obviously, the linearization (5.13) implies

$$\bar{\phi} = \phi(\bar{x}) = \frac{1}{n}\sum_{l=1}^{n} \phi(x_l)\,. \tag{5.16}$$

Using (5.13), the empirical variance of the $\phi(x_l)$ with respect to their mean $\phi(\bar{x})$ is given by

$$s_\phi^2 = \frac{1}{n-1}\sum_{l=1}^{n} \left[\phi(x_l) - \phi(\bar{x})\right]^2 = \left(\frac{\mathrm{d}\phi}{\mathrm{d}\bar{x}}\right)^2 s_x^2\,. \tag{5.17}$$

If the x_l are normally distributed, this holds also for the $\phi(x_l)$, $l = 1, \ldots, n$. Hence, referring to (5.12), (5.14) and (5.17), we are in a position to define a Student's

[2] abbreviating the operation of differentiation.

$$T(n-1) = \frac{\phi(\bar{X}) - \mu_\phi}{S_\phi/\sqrt{n}}$$

through

$$T(n-1) = \frac{\dfrac{\mathrm{d}\phi}{\mathrm{d}\bar{x}}(\bar{X} - \mu_x)}{\left|\dfrac{\mathrm{d}\phi}{\mathrm{d}\bar{x}}\right| \dfrac{S_x}{\sqrt{n}}} = \operatorname{sign}\left(\frac{\mathrm{d}\phi}{\mathrm{d}\bar{x}}\right) \frac{(\bar{X} - \mu_x)}{S_x/\sqrt{n}}\,, \tag{5.18}$$

where the sign function is meaningless on account of the symmetry of Student's density. After all, (5.18) provides a confidence interval

$$\phi(\bar{X}) \pm \frac{t_P(n-1)}{\sqrt{n}}\, S_\phi \tag{5.19}$$

for the parameter μ_ϕ with reference to a confidence level P. Combining (5.19) with the worst case estimate

$$f_{s,\phi} = \left|\frac{\mathrm{d}\phi}{\mathrm{d}\bar{x}}\right| f_{s,x}\,; \quad -f_{s,\phi} \le f_\phi \le f_{s,\phi} \tag{5.20}$$

of the propagated systematic error f_ϕ, the overall uncertainty turns out to be

$$u_\phi = \left|\frac{\mathrm{d}\phi}{\mathrm{d}\bar{x}}\right| \left[\frac{t_P(n-1)}{\sqrt{n}}\, s_x + f_{s,x}\right] = \left|\frac{\mathrm{d}\phi}{\mathrm{d}\bar{x}}\right| u_{\bar{x}}\,, \tag{5.21}$$

where $u_{\bar{x}}$ is given in (5.10). Thus, the final measurement result is

$$\phi(\bar{x}) \pm u_{\bar{\phi}}\,. \tag{5.22}$$

Examples

(i) Occasionally, the fine structure constant[3]

$$\bar{\alpha} = 7.29735308(33)\,10^{-3}$$

is inversely written

$$\bar{\alpha}^{-1} = 137.03598949\cdots\,.$$

We shall determine the uncertainty $u_{\bar{\alpha}^{-1}}$, given $u_{\bar{\alpha}} = t_P s_\alpha/\sqrt{n} + f_{s,\alpha}$.

Linearizing $\phi(\alpha) = 1/\alpha$,

$$\phi(\alpha_l) - \phi(\bar{\alpha}) = -\frac{1}{\bar{\alpha}^2}(\alpha_l - \bar{\alpha})\,; \quad l = 1\,, \ldots,\, n$$

[3]The data are taken from [17]. Here, the rounding procedures proposed in Sect. 1.2 do not apply. Instead, uncertainties are generally provided with two digits.

we find

$$s^2_{\alpha^{-1}} = \frac{1}{\bar{\alpha}^4} s^2_\alpha \,.$$

As

$$f_{\alpha^{-1}} = -\frac{1}{\bar{\alpha}^2} f_\alpha \,,$$

the uncertainty in question is

$$u_{\bar{\alpha}^{-1}} = \frac{1}{\bar{\alpha}^2} \left[\frac{t_P}{\sqrt{n}}\, s_\alpha + f_{s,\alpha} \right] = \frac{u_{\bar{\alpha}}}{\bar{\alpha}^2}$$

so that

$$\bar{\alpha}^{-1} = 137.0359895(62) \,.$$

We notice that the relative uncertainties are equal,

$$\frac{u_{\bar{\alpha}^{-1}}}{\bar{\alpha}^{-1}} = \frac{u_{\bar{\alpha}}}{\bar{\alpha}} \,.$$

The same applies when ppm are introduced. As

$$\frac{u_{\mathrm{ppm},\,\bar{\alpha}}}{10^6} = \frac{u_{\bar{\alpha}}}{\bar{\alpha}} \,,$$

we have

$$u_{\mathrm{ppm},\,\bar{\alpha}} = \frac{u_{\bar{\alpha}}}{\bar{\alpha}} 10^6 = \frac{u_{\bar{\alpha}^{-1}}}{\bar{\alpha}^{-1}} 10^6 = u_{\mathrm{ppm},\,\bar{\alpha}^{-1}} = 0.045 \,.$$

(ii) Given the uncertainty $u_{\bar{c}}$ of the correction $\bar{c}$ to the base unit ampere, $1\,\mathrm{A} = (1\,\mathrm{A_L} + \bar{c}) \pm u_{\bar{c}}$, we shall find the uncertainty of the conversion factor K_A.

Setting $K_\mathrm{A} = y$ and $\{c\} = x$ so that $y = 1/(1+x)$, we obtain

$$\bar{y} - y_0 = \frac{\mathrm{d}y}{\mathrm{d}x_0}(\bar{x} - x_0) \,; \quad \bar{x} - x_0 = (\bar{x} - \mu_x) + f_x$$

i.e.

$$\bar{y} - y_0 = \frac{\mathrm{d}y}{\mathrm{d}x_0} \left[(\bar{x} - \mu_x) + f_x \right] \,.$$

But then

$$u_{\bar{y}} = \left| \frac{\mathrm{d}y}{\mathrm{d}\bar{x}} \right| \left[\frac{t_P}{\sqrt{n}}\, s_x + f_{s,x} \right]$$

or

$$u_{\bar{K}_\mathrm{A}} = \frac{u_{\{\bar{c}\}}}{(1 + \{\bar{c}\})^2} \,.$$

Just to illustrate the situation, let us refer to the 1986 adjustment of the fundamental physical constants [17]. We have

$$K_{\mathrm{A}} = 0.99999397 \pm 0.3 \times 10^{-6} .$$

This means

$$\begin{aligned} 1\mathrm{A}_{\mathrm{L}} &= K_{\mathrm{A}}\, 1\mathrm{A} = 0.99999397\,\mathrm{A} \\ \{\bar{c}\} &= 6.03 \times 10^{-6} \\ u_{\{\bar{c}\}} &= 0.30 \times 10^{-6}\,\mathrm{A} \\ \bar{c} &= 6.03 \times 10^{-6}\,\mathrm{A}_{\mathrm{L}} , \end{aligned}$$

so that

$$1\mathrm{A}_{\mathrm{L}} + \bar{c} = 0.99999397 + 0.00000603 = 1\,\mathrm{A} .$$

In Sect. 6.4 we shall assess the uncertainty $u_{\bar{c}}$, given $u_{\bar{a}}$ and $u_{\bar{b}}$. Furthermore, given $u_{\bar{\mathrm{V}}}$ and $u_{\bar{K}_\Omega}$, we shall quote the uncertainty $u_{\bar{K}_{\mathrm{A}}}$.

5.4 Systematic Errors of the Measurands

Should the measurand itself for any reason be blurred, a true value x_0 would not exist. Even in this case it would, however, be assumed that the measurand remains constant during the time it takes to perform n repeat measurements. The blurry structure of the measurand can be taken into account by an additional systematic error

$$-f_{s,x_0} \le f_{x_0} \le f_{s,x_0} . \tag{5.23}$$

The linewidths on semiconductor templates, for example, may locally vary more or less severely. Subject to the resolution of the measuring process, such variations will be integrated out or disclosed. If integrated out, an additional systematic error should account for the inconstancies of the linewidths.

The extra systematic error f_{x_0} of the measurand may be merged with the systematic error of the measuring process

$$-f_{s,x} \le f_x \le f_{s,x}$$

into an overall systematic error

$$-(f_{s,x} + f_{s,x_0}), \ldots, (f_{s,x} + f_{s,x_0}) . \tag{5.24}$$

It is essential that during the time it takes to register the repeat measurements $f_x = \text{const.}$ and $f_{x_0} = \text{const.}$

The formalization of series of measurements which are subject to time-varying systematic errors giving rise to so-called time series would be outside the scope of this presentation. A basic metrological example is given in [12].

6 Propagation of Measurement Errors

6.1 Taylor Series Expansion

We consider a functional relationship $\phi(x, y)$ and given results of measurement

$$\bar{x} \pm u_{\bar{x}} \quad \text{and} \quad \bar{y} \pm u_{\bar{y}} \tag{6.1}$$

localizing true values x_0 and y_0 respectively. The latter define a quantity $\phi(x_0, y_0)$ which we regard as the true value of the physical quantity in question. The result to be found,

$$\phi(\bar{x}, \bar{y}) \pm u_{\bar{\phi}}\,, \tag{6.2}$$

should localize this quantity $\phi(x_0, y_0)$. In general, it is sufficient to base the assessment of the uncertainty $u_{\bar{\phi}}$ on the linear part of the Taylor expansion. Within the scope of this approximation and due to the error model relied on, the error propagation resolves into two different, independent branches covering the propagation of random and systematic errors.

Expanding $\phi(x_l, y_l)$; $l = 1, 2, \ldots, n$ throughout a neighborhood of the point x_0, y_0,

$$\phi(x_l, y_l) = \phi(x_0, y_0) + \left.\frac{\partial \phi}{\partial x}\right|_{\substack{x = x_0 \\ y = y_0}} (x_l - x_0) + \left.\frac{\partial \phi}{\partial y}\right|_{\substack{x = x_0 \\ y = y_0}} (y_l - y_0) + \cdots$$

and referring to the error equations

$$x_l = x_0 + (x_l - \mu_x) + f_x, \quad y_l = y_0 + (y_l - \mu_y) + f_y \tag{6.3}$$

yields[1]

$$\begin{aligned} \phi(x_l, y_l) = {} & \phi(x_0, y_0) \\ & + \left[\frac{\partial \phi}{\partial \bar{x}}(x_l - \mu_x) + \frac{\partial \phi}{\partial \bar{y}}(y_l - \mu_y)\right] + \left[\frac{\partial \phi}{\partial \bar{x}} f_x + \frac{\partial \phi}{\partial \bar{y}} f_y\right]. \end{aligned} \tag{6.4}$$

[1] abbreviating the operation of differentiation.

For the sake of lucidity, the truncated series expansion has been expressed in terms of an equality, which, of course, is incorrect. By approximation, we shall treat the differential quotients as constants – this will keep the formalism controllable. As we assume equal numbers of repeat measurements, we may sum over l and divide by n. Subtracting

$$\begin{aligned}\phi(\bar{x},\bar{y}) &= \phi(x_0,y_0) \\ &+ \left[\frac{\partial\phi}{\partial\bar{x}}(\bar{x}-\mu_x)+\frac{\partial\phi}{\partial\bar{y}}(\bar{y}-\mu_y)\right]+\left[\frac{\partial\phi}{\partial\bar{x}}f_x+\frac{\partial\phi}{\partial\bar{y}}f_y\right]\end{aligned} \tag{6.5}$$

from (6.4) we find

$$\phi(x_l,y_l)-\phi(\bar{x},\bar{y})=\frac{\partial\phi}{\partial\bar{x}}(x_l-\bar{x})+\frac{\partial\phi}{\partial\bar{y}}(y_l-\bar{y}) \tag{6.6}$$

The linearization implies

$$\bar{\phi}=\frac{1}{n}\sum_{l=1}^{n}\phi(x_l,y_l)=\phi(\bar{x},\bar{y})\,. \tag{6.7}$$

From the expectation

$$\mu_\phi=E\left\{\phi(\bar{X},\bar{Y})\right\}=\phi(x_0,y_0)+\left[\frac{\partial\phi}{\partial\bar{x}}f_x+\frac{\partial\phi}{\partial\bar{y}}f_y\right] \tag{6.8}$$

we seize:

The unknown systematic errors f_x and f_y cause the expectation μ_ϕ of the arithmetic mean $\phi(\bar{X},\bar{Y})$ to be biased with respect to the true value $\phi(x_0,y_0)$.

The bias is the propagated systematic error

$$f_\phi=\frac{\partial\phi}{\partial\bar{x}}f_x+\frac{\partial\phi}{\partial\bar{y}}f_y\,;\quad -f_{s,x}\le f_x\le f_{s,x}\,,\quad -f_{s,y}\le f_y\le f_{s,y}\,. \tag{6.9}$$

The uncertainty $u_{\bar{\phi}}$ sought-for will be assessed by means of (6.6) and (6.9). Let us summarize. On account of the error model, the linear part of the Taylor expansion (6.5) splits up into two terms. The part due to random errors embodies the unknown expectations μ_x,μ_y. As a result, no direct assessment is possible. Meanwhile the difference (6.6) will help us to overcome the difficulty. In contrast to this, the second term of (6.5) which expresses the influence of systematic errors, turns out to be directly assessable.

Finally, for formal reasons, we define the vectors

$$\boldsymbol{b}=\begin{pmatrix}\dfrac{\partial\phi}{\partial\bar{x}}\\[2ex]\dfrac{\partial\phi}{\partial\bar{y}}\end{pmatrix}\,,\quad \bar{\boldsymbol{\zeta}}-\boldsymbol{\mu}=\begin{pmatrix}\bar{x}-\mu_x\\[2ex]\bar{y}-\mu_y\end{pmatrix} \tag{6.10}$$

so that (6.5) changes into

$$\phi(\bar{x}, \bar{y}) = \mu_\phi + \boldsymbol{b}^{\mathrm{T}}(\bar{\boldsymbol{\zeta}} - \boldsymbol{\mu})\,. \tag{6.11}$$

To set up the error propagation for more than two variables, we generalize the nomenclature. We consider a functional relationship $\phi(x_1, x_2, \ldots, x_m)$ and arithmetic means

$$\bar{x}_i = \frac{1}{n}\sum_{l=1}^{n} x_{il}\,; \quad i = 1, 2\,, \ldots,\, m \tag{6.12}$$

to be based on an identical number n of repeat measurements.

As usual, we designate the true values of the measurands $\bar{x}_i$; $i = 1, 2, \ldots, m$ by

$$x_{0,1},\, x_{0,2}\,, \ldots,\, x_{0,m}\,. \tag{6.13}$$

Then, the final result

$$\phi(\bar{x}_1, \bar{x}_2\,, \ldots,\, \bar{x}_m) \pm u_{\bar{\phi}} \tag{6.14}$$

should localize the true value $\phi(x_{0,1}, x_{0,2}, \ldots, x_{0,m})$. In analogy to (6.5), we have

$$\phi(\bar{x}_1, \bar{x}_2, \ldots \bar{x}_m) = \mu_\phi + \sum_{i=1}^{m} \frac{\partial \phi}{\partial \bar{x}_i}(\bar{x}_i - \mu_i)\,; \quad \mu_i = E\{\bar{X}_i\}\,, \tag{6.15}$$

where

$$\begin{aligned} \mu_\phi &= E\left\{\phi(\bar{X}_1, \bar{X}_2, \ldots, \bar{X}_m)\right\} \\ &= \phi(x_{0,1}, x_{0,2}, \ldots, x_{0,m}) + \sum_{i=1}^{m} \frac{\partial \phi}{\partial \bar{x}_i} f_i\,. \end{aligned} \tag{6.16}$$

The contribution

$$f_\phi = \sum_{i=1}^{m} \frac{\partial \phi}{\partial \bar{x}_i} f_i\,; \quad -f_{s,i} \le f_i \le f_{s,i} \tag{6.17}$$

denotes the propagated systematic error biasing the true value $\phi(x_{0,1}, x_{0,2}$, $\ldots, x_{0,m})$. Instead of (6.6) we here have, letting $l = 1, 2, \ldots, n$,

$$\phi(x_{1l}, x_{2l}, \ldots x_{ml}) - \phi(\bar{x}_1, \bar{x}_2, \ldots \bar{x}_m) = \sum_{i=1}^{m} \frac{\partial \phi}{\partial \bar{x}_i}(x_{il} - \bar{x}_i)\,. \tag{6.18}$$

Finally, we convert (6.15) into vector form

$$\phi(\bar{x}_1, \bar{x}_2, \ldots \bar{x}_m) = \mu_\phi + \boldsymbol{b}^{\mathrm{T}}(\bar{\boldsymbol{x}} - \boldsymbol{\mu})\,, \tag{6.19}$$

where

$$\boldsymbol{b} = \left[\frac{\partial \phi}{\partial \bar{x}_1} \; \cdots \; \frac{\partial \phi}{\partial \bar{x}_m} \right]^{\mathrm{T}}$$

and

$$\bar{\boldsymbol{x}} - \boldsymbol{\mu} = (\bar{x}_1 - \mu_1 \; \cdots \; \bar{x}_m - \mu_m)^{\mathrm{T}} .$$

We are ultimately prepared to reformulate the formalism for error propagation.

6.2 Expectation of the Arithmetic Mean

We might wish to assess the statistical fluctuations of the random errors from (6.4) and (6.8),

$$\phi(x_l, y_l) = \mu_\phi + \left[\frac{\partial \phi}{\partial \bar{x}} (x_l - \mu_x) + \frac{\partial \phi}{\partial \bar{y}} (y_l - \mu_y) \right] ; \quad l = 1, 2, \ldots, n \tag{6.20}$$

by means of the expectation

$$\begin{aligned} \sigma_\phi^2 &= E\left\{ (\phi(X, Y) - \mu_\phi)^2 \right\} \\ &= \left(\frac{\partial \phi}{\partial \bar{x}} \right)^2 \sigma_x^2 + 2 \left(\frac{\partial \phi}{\partial \bar{x}} \right) \left(\frac{\partial \phi}{\partial \bar{y}} \right) \sigma_{xy} + \left(\frac{\partial \phi}{\partial \bar{x}} \right)^2 \sigma_y^2 . \end{aligned} \tag{6.21}$$

However, neither the theoretical variances nor the theoretical covariance are available – the latter may turn out to be positive or negative. Resorting to (6.6), we can overcome the problem that we do not know the theoretical moments of second order, as

$$\phi(x_l, y_l) - \phi(\bar{x}, \bar{y}) = \frac{\partial \phi}{\partial \bar{x}} (x_l - \bar{x}) + \frac{\partial \phi}{\partial \bar{y}} (y_l - \bar{y}) ; \quad l = 1, 2, \ldots, n$$

puts us in a position to express the scattering of the random errors via the empirical moments,

$$s_x^2 , \quad s_{xy} \quad \text{and} \quad s_y^2$$

so that

$$s_\phi^2 = \frac{1}{n-1} \sum_{l=1}^{n} [\phi(x_l, y_l) - \phi(\bar{x}, \bar{y})]^2$$

yields

$$s_\phi^2 = \frac{1}{n-1}\sum_{l=1}^{n}\left[\left(\frac{\partial\phi}{\partial\bar{x}}\right)^2(x_l-\bar{x})^2\right.$$

$$\left.+2\left(\frac{\partial\phi}{\partial\bar{x}}\right)\left(\frac{\partial\phi}{\partial\bar{y}}\right)(x_l-\bar{x})(y_l-\bar{y})+\left(\frac{\partial\phi}{\partial\bar{y}}\right)^2(y_l-\bar{y})^2\right]$$

$$=\left(\frac{\partial\phi}{\partial\bar{x}}\right)^2 s_x^2+2\left(\frac{\partial\phi}{\partial\bar{x}}\right)\left(\frac{\partial\phi}{\partial\bar{y}}\right)s_{xy}+\left(\frac{\partial\phi}{\partial\bar{y}}\right)^2 s_y^2\,. \tag{6.22}$$

As the empirical variances s_x^2, s_y^2 and the empirical covariance s_{xy} are unbiased, the random variable S_ϕ^2 is unbiased as well, $E\{S_\phi^2\}=\sigma_\phi^2$.

Succeeding pairs $x_1,y_1;x_2,y_2;\ldots;x_n,y_n$ are independent. On the other hand, with respect to the same l, x_l and y_l may well be dependent. When the pairs x_l,y_l are assigned to the random variables X,Y of a two-dimensional normal probability density, the quantities $\phi(x_l,y_l);l=1,2,\ldots,n$ defined in (6.20) are normally distributed, be X and Y dependent or not. However, succeeding pairs $\phi(x_l,y_l);\phi(x_{l+1},y_{l+1})$ are independent, like pairs x_l,y_l; x_{l+1},y_{l+1}. As s_ϕ^2 estimates σ_ϕ^2, we are in a position to define a

$$\chi^2(n-1)=\frac{(n-1)S_\phi^2}{\sigma_\phi^2} \tag{6.23}$$

and a Student's

$$T(n-1)=\frac{\phi(\bar{X},\bar{Y})-\mu_\phi}{S_\phi/\sqrt{n}}\,. \tag{6.24}$$

They are defined because we have agreed on statistically well-defined measuring conditions. Thus,

$$\phi(\bar{X},\bar{Y})-\frac{t_P(n-1)}{\sqrt{n}}\,S_\phi\le\mu_\phi\le\phi(\bar{X},\bar{Y})+\frac{t_P(n-1)}{\sqrt{n}}\,S_\phi \tag{6.25}$$

is a confidence interval for the expectation μ_ϕ of the arithmetic mean $\phi(\bar{X},\bar{Y})$. The subscript P in t_P specifies the associated level of confidence. Seen experimentally we state:

The confidence interval

$$\phi(\bar{x},\bar{y})\pm\frac{t_P(n-1)}{\sqrt{n}}\,s_\phi \tag{6.26}$$

localizes the expected value $\mu_\phi=E\{\phi(\bar{X},\bar{Y})\}$ of the random variable $\phi(\bar{X},\bar{Y})$ *with probability* $P\{t_P(n-1)\}$.

Referring to the empirical variance–covariance matrix

$$s=\begin{pmatrix}s_{xx} & s_{xy}\\ s_{yx} & s_{yy}\end{pmatrix};\quad s_{xx}\equiv s_x^2,\quad s_{xy}=s_{yx},\quad s_{yy}\equiv s_y^2$$

and the vector $\boldsymbol{b}$ defined in (6.10), we may compress (6.22) into

$$s_\phi^2 = \boldsymbol{b}^{\mathrm{T}} \boldsymbol{s}\, \boldsymbol{b}\,. \tag{6.27}$$

The formalism does not require us to differentiate between dependent and independent random variables. In the case of a dependence, the experimental device watches out which realizations of X and Y fit together. In the case of independence, the experimenter may realize any ordering.[2] The numerical value of the empirical covariance s_{xy} depends on the kind of pairing chosen. While all the values are equally well admissible, each of them is confined to the interval

$$-s_x s_y \le s_{xy} \le s_x s_y\,.$$

Even purposeful modifications of the data ordering would not invalidate (6.26).

The conventional error calculus, ignoring empirical covariances, restricts itself to empirical variances and, dividing them by their respective numbers of repeat measurements, defines a quantity

$$s_{\bar\phi}^* = \sqrt{\left(\frac{\partial\phi}{\partial\bar x}\right)^2 \frac{s_x^2}{n_x} + \left(\frac{\partial\phi}{\partial\bar x}\right)^2 \frac{s_y^2}{n_y}}$$

ad hoc. With reference to B.L. Welch's effective degrees of freedom ν_{eff}, a confidence region approximating Student's interval (6.26) can still be given [7]

$$\phi(\bar x, \bar y) - t_P(\nu_{\mathrm{eff}}) s_{\bar\phi}^* \le \mu_\phi \le \phi(\bar x, \bar y) + t_P(\nu_{\mathrm{eff}}) s_{\bar\phi}^*\,.$$

For more than two variables, little is to be added. From (6.18) we derive the empirical variance

$$s_\phi^2 = \sum_{i,j}^{m} \frac{\partial\phi}{\partial\bar x_i} \frac{\partial\phi}{\partial\bar x_j} s_{ij} = \boldsymbol{b}^{\mathrm{T}} \boldsymbol{s}\, \boldsymbol{b}\,, \tag{6.28}$$

in which the vector $\boldsymbol{b}$ and the matrix $\boldsymbol{s}$ are given by

$$\boldsymbol{b} = \left(\frac{\partial\phi}{\partial\bar x_1}\ \frac{\partial\phi}{\partial\bar x_2}\ \cdots\ \frac{\partial\phi}{\partial\bar x_m}\right)^{\mathrm{T}} \tag{6.29}$$

and

$$\boldsymbol{s} = \begin{pmatrix} s_{11} & s_{12} & \dots & s_{1m} \\ s_{21} & s_{22} & \dots & s_{2m} \\ \dots & \dots & \dots & \dots \\ s_{m1} & s_{m2} & \dots & s_{mm} \end{pmatrix}$$

[2] For example, the two series $(x_1, y_1), (x_2, y_2), \dots$ and $(x_1, y_2), (x_2, y_1), \dots$ would be equally admissible.

$$s_{ij} = \frac{1}{n-1}\sum_{l=1}^{n}(x_{il} - \bar{x}_i)(x_{jl} - \bar{x}_j)\,; \quad i,j = 1\,,\ldots,\,m \tag{6.30}$$

respectively. If need be, we shall denote the diagonal elements of $\boldsymbol{s}$ as $s_{ii} \equiv s_i^2$. Furthermore, for reasons of symmetry, we have $s_{ij} = s_{ji}$. Finally, Student's confidence interval for the parameter μ_ϕ which has been defined in (6.16) turns out to be

$$\phi(\bar{X}_1, \bar{X}_2, \ldots, \bar{X}_m) \pm \frac{t_P(n-1)}{\sqrt{n}} S_\phi\,. \tag{6.31}$$

To assess the influence of systematic errors, we shall have to refer to (6.9) and (6.17).

6.3 Uncertainty of the Arithmetic Mean

According to (6.8), the expectation μ_ϕ differs from the true value $\phi(x_0, y_0)$ by the propagated systematic error

$$f_\phi = \frac{\partial\phi}{\partial\bar{x}} f_x + \frac{\partial\phi}{\partial\bar{y}} f_y\,; \quad -f_{s,x} \le f_x \le f_{s,x}\,; \quad -f_{s,y} \le f_y \le f_{s,y}\,, \tag{6.32}$$

where neither the signs nor the magnitudes of f_x and f_y are known. As we wish to safely localize the true value $\phi(x_0, y_0)$, we opt for a worst case estimation, setting

$$f_{s,\phi} = \left|\frac{\partial\phi}{\partial\bar{x}}\right| f_{s,x} + \left|\frac{\partial\phi}{\partial\bar{y}}\right| f_{s,y} \tag{6.33}$$

and quote the result of measurement as

$$\phi(\bar{x}, \bar{y}) \pm u_{\bar{\phi}}$$

$$u_{\bar{\phi}} = \frac{t_P(n-1)}{\sqrt{n}} \sqrt{\left(\frac{\partial\phi}{\partial\bar{x}}\right)^2 s_x^2 + 2\left(\frac{\partial\phi}{\partial\bar{x}}\right)\left(\frac{\partial\phi}{\partial\bar{y}}\right) s_{xy} + \left(\frac{\partial\phi}{\partial\bar{y}}\right)^2 s_y^2}$$

$$+ \left|\frac{\partial\phi}{\partial\bar{x}}\right| f_{s,x} + \left|\frac{\partial\phi}{\partial\bar{y}}\right| f_{s,y}\,. \tag{6.34}$$

We do not assign a probability to this statement. Considering m variables, we have

$$\phi(\bar{x}_1, \bar{x}_2, \ldots, \bar{x}_m) \pm u_{\bar{\phi}}$$

$$u_{\bar{\phi}} = \frac{t_P(n-1)}{\sqrt{n}} \sqrt{\sum_{i,j}^{m} \frac{\partial\phi}{\partial\bar{x}_i}\frac{\partial\phi}{\partial\bar{x}_j} s_{ij}} + \sum_{i=1}^{m}\left|\frac{\partial\phi}{\partial\bar{x}_i}\right| f_{s,i}\,, \tag{6.35}$$

expecting the so-defined interval to localize the true value $\phi(x_{0,1}, x_{0,2}, \ldots, x_{0,m})$.

The question as to whether worst case estimations of propagated systematic errors might provoke unnecessarily large uncertainties or whether the relevant *ISO Guide's* quadratic estimations might, in the end, lead to unreliably small uncertainties, is still controversial. Here, worst case estimations and a linear combination of random and systematic errors are in any case preferred in contrast to the *Guide* which, postulating theoretical variances for systematic errors, adds uncertainty components quadratically. The computer simulations in the next section will serve to scrutinize the differences.

There are useful supplements to (6.34) and (6.35). Remarkably enough, as $-s_x s_y \le s_{xy} \le s_x s_y$, the term due to random errors can be reduced as follows

$$\begin{aligned}
&\left(\frac{\partial\phi}{\partial\bar{x}}\right)^2 s_x^2 + 2\left(\frac{\partial\phi}{\partial\bar{x}}\right)\left(\frac{\partial\phi}{\partial\bar{y}}\right) s_{xy} + \left(\frac{\partial\phi}{\partial\bar{y}}\right)^2 s_y^2 \\
&\le \left(\frac{\partial\phi}{\partial\bar{x}}\right)^2 s_x^2 + 2\left|\frac{\partial\phi}{\partial\bar{x}}\right|\left|\frac{\partial\phi}{\partial\bar{y}}\right| s_x s_y + \left(\frac{\partial\phi}{\partial\bar{y}}\right)^2 s_y^2 \\
&= \left(\left|\frac{\partial\phi}{\partial\bar{x}}\right| s_x + \left|\frac{\partial\phi}{\partial\bar{y}}\right| s_y\right)^2 \qquad (6.36)
\end{aligned}$$

so that (6.34) simplifies to

$$\begin{aligned}
u_{\bar{\phi}} &= \frac{t_P(n-1)}{\sqrt{n}}\sqrt{\left(\frac{\partial\phi}{\partial\bar{x}}\right)^2 s_x^2 + 2\left(\frac{\partial\phi}{\partial\bar{x}}\right)\left(\frac{\partial\phi}{\partial\bar{y}}\right) s_{xy} + \left(\frac{\partial\phi}{\partial\bar{y}}\right)^2 s_y^2} \\
&\quad + \left|\frac{\partial\phi}{\partial\bar{x}}\right| f_{s,x} + \left|\frac{\partial\phi}{\partial\bar{y}}\right| f_{s,y} \\
&\le \left|\frac{\partial\phi}{\partial\bar{x}}\right|\left(\frac{t_P(n-1)}{\sqrt{n}} s_x + f_{s,x}\right) + \left|\frac{\partial\phi}{\partial\bar{y}}\right|\left(\frac{t_P(n-1)}{\sqrt{n}} s_y + f_{s,y}\right) \\
&= \left|\frac{\partial\phi}{\partial\bar{x}}\right| u_{\bar{x}} + \left|\frac{\partial\phi}{\partial\bar{y}}\right| u_{\bar{y}}\,,
\end{aligned}$$

i.e.

$$u_{\bar{\phi}} \le \left|\frac{\partial\phi}{\partial\bar{x}}\right| u_{\bar{x}} + \left|\frac{\partial\phi}{\partial\bar{y}}\right| u_{\bar{y}}\,. \qquad (6.37)$$

Obviously, it is of no significance that this expression is based upon a singular empirical variance–covariance matrix $\boldsymbol{s}$.

A corresponding simplification is available for (6.35): considering two variables at a time, the respective empirical covariance may be treated just as in the case of two variables. But this leads to

$$u_{\bar{\phi}} \leq \sum_{i=1}^{m} \left| \frac{\partial \phi}{\partial \bar{x}_i} \right| u_{\bar{x}_i} \,. \tag{6.38}$$

In a sense, this approach conceals the empirical covariances between the variables, saving us the necessity to calculate them afterwards from raw data, if need be. Evidently, just this latter property renders (6.38) particularly attractive. With this, we finish the development of the new formalism of error propagation. Its basic principles rely on

- stationarily operated non-drifting measuring devices,
- decoupled random and systematic errors,
- linearized Taylor series expansion,
- well-defined measuring conditions,
- the propagation of random errors via Student's confidence intervals and systematic errors by means of worst case estimations, and
- the linear combination of the uncertainty components due to random and systematic errors.

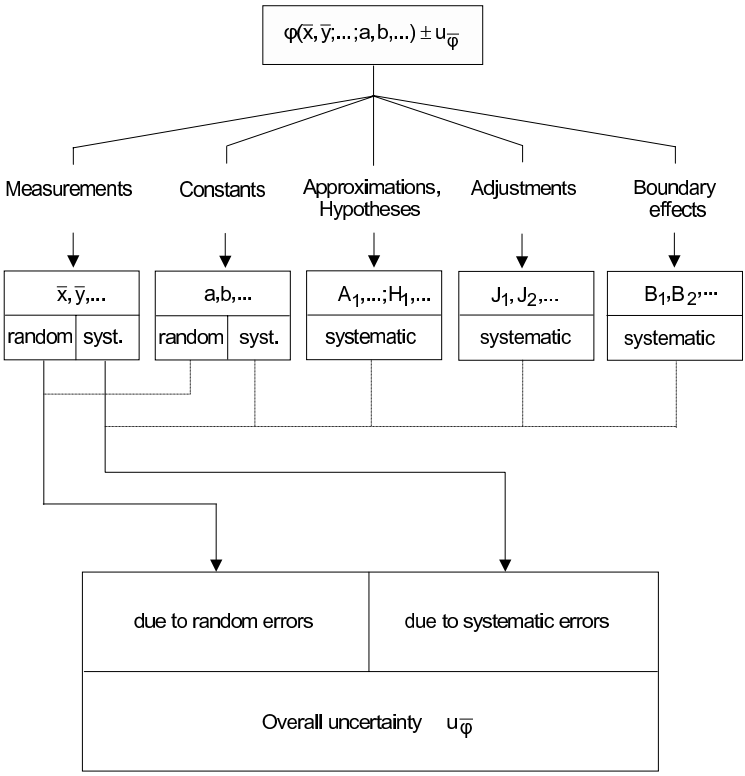


Fig. 6.1. Flow of random and systematic errors

Figure 6.1 presents a descriptive overview of the origin, the classification and the flow of errors entering measurement uncertainties.

The errors of physical constants have to be treated according to the particular role they play in the measuring process under consideration. If constants, akin to measurands, appear as arguments of functional relationships, their uncertainty components should be broken up into components according to whether they are of random or systematic origin. If, on the other hand, they are physically active parts of the measuring procedure applying for example to material measures, their uncertainties will exclusively be effective as systematic errors. An example will be given in Sect. 12.5.

In general, error propagation covers several stages. As will be shown in Sect. 6.5, the error model under discussion steadily channels the flow of random and systematic errors.

6.4 Uncertainties of Elementary Functions

We shall illustrate the new formalism by means of some examples.

Sums and Differences

Given two measurands x and y, we combine the results

$$\bar{x} \pm \left(\frac{t_P(n-1)}{\sqrt{n}} s_x \right) \quad \text{and} \quad \bar{y} \pm \left(\frac{t_P(n-1)}{\sqrt{n}} s_y \right) \tag{6.39}$$

to form functional relationships

$$\phi(x, y) = x \pm y \,. \tag{6.40}$$

With respect to the sum, $\phi(x, y) = x + y$, the error equations yield

$$\phi(x_l, y_l) = x_0 + y_0 + (x_l - \mu_x) + (y_l - \mu_y) + f_x + f_y \tag{6.41}$$

and

$$\phi(\bar{x}, \bar{y}) = x_0 + y_0 + (\bar{x} - \mu_x) + (\bar{y} - \mu_y) + f_x + f_y \tag{6.42}$$

respectively. Then, subtracting (6.41) and (6.42), we obtain

$$\phi(x_l, y_l) - \phi(\bar{x}, \bar{y}) = (x_l - \bar{x}) + (y_l - \bar{y}) \,. \tag{6.43}$$

The expected value of (6.41),

$$\mu_\phi = E\{\phi(X, Y)\} = x_0 + y_0 + f_x + f_y \tag{6.44}$$

reveals a propagated systematic error

$$f_\phi = f_x + f_y\,; \quad -f_{s,x} \le f_x \le f_{s,x}\,; \quad -f_{s,y} \le f_x \le f_{s,y}\,. \tag{6.45}$$

Furthermore, from (6.43) we obtain an estimator

$$s_\phi^2 = \frac{1}{n-1}\sum_{l=1}^{n}\left[\phi(x_l, y_l) - \phi(\bar{x}, \bar{y})\right]^2 = s_x^2 + 2s_{xy} + s_y^2 \tag{6.46}$$

for the theoretical variance $\sigma_\phi^2 = E\{(\phi(X,Y) - \mu_\phi)^2\}$ so that the final result is

$$\phi(\bar{x}, \bar{y}) \pm u_{\bar{\phi}}$$

$$u_{\bar{\phi}} = \frac{t_P(n-1)}{\sqrt{n}}\sqrt{s_x^2 + 2s_{xy} + s_y^2} + (f_{s,x} + f_{s,y})\,. \tag{6.47}$$

Now, in terms of a test of hypothesis, we ask for the compatibility of two arithmetic means, $\bar{x}$ and $\bar{y}$ aiming at one and the same physical quantity, i.e. we are looking for a maximum tolerable deviation $|\bar{x} - \bar{y}|$. Setting

$$\phi(x_l, y_l) - \phi(\bar{x}, \bar{y}) = (x_l - \bar{x}) - (y_l - \bar{y}) \tag{6.48}$$

we find

$$s_\phi^2 = s_x^2 - 2s_{xy} + s_y^2 \tag{6.49}$$

and, as

$$f_\phi = f_x - f_y\,; \quad -f_{s,x} \le f_x \le f_{s,x}\,; \quad -f_{s,y} \le f_x \le f_{s,y}\,, \tag{6.50}$$

these two means are compatible if

$$|\bar{x} - \bar{y}| \le \frac{t_p(n-1)}{\sqrt{n}}\sqrt{s_x^2 - 2s_{xy} + s_y^2} + (f_{s,x} + f_{s,y})\,. \tag{6.51}$$

Condoning a singular empirical variance–covariance matrix, a coarser estimation would be

$$|\bar{x} - \bar{y}| \le u_{\bar{x}} + u_{\bar{y}}\,. \tag{6.52}$$

Within the scope of so-called round robins, Sect. 12.1, one and the same measuring object is circulated amongst various laboratories. Each of the participants measures the same physical quantity. Assuming this quantity remains constant during the whole period of circulation, then, any two uncertainties taken at a time should mutually overlap.

Example

We estimate the uncertainty $u_{\bar{c}}$ of the correction $\bar{c}$ to the ampere, given the uncertainties $u_{\bar{a}}$ and $u_{\bar{b}}$ of the corrections $\bar{a}$ and $\bar{b}$ to the volt and the ohm.

In Sect. 5.2 we had $1\,\mathrm{V} = (1 + \{\bar{a}\})\,\mathrm{V_L}$; $1\,\Omega = (1 + \{\bar{b}\})\,\Omega_\mathrm{L}$; $1\,\mathrm{A} = (1 + \{\bar{c}\})\,\mathrm{A_L}$. From

$$\{c\} = \{a\} - \{b\}$$

we deduce

$$u_{\{\bar{c}\}} = \frac{t_P(n-1)}{\sqrt{n}} \sqrt{s^2_{\{a\}} - 2s_{\{a\}\{b\}} + s^2_{\{b\}}} + (f_{s,\{a\}} + f_{s,\{b\}})\,.$$

Products and Quotients

Linearizing the product

$$\phi(x, y) = xy \tag{6.53}$$

yields

$$\phi(x_l, y_l) - \phi(\bar{x}, \bar{y}) = \bar{y}(x_l - \bar{x}) + \bar{x}(y_l - \bar{y})\,; \quad l = 1, 2\,, \ldots,\, n$$

so that

$$s^2_\phi = \bar{y}^2 s^2_x + 2\,\bar{x}\,\bar{y}\,s_{xy} + \bar{x}^2 s^2_y\,. \tag{6.54}$$

As

$$f_\phi = \bar{y} f_x + \bar{x} f_y\,, \tag{6.55}$$

we have

$$f_{s,\phi} = |\bar{y}| f_{s,x} + |\bar{x}| f_{s,y} \tag{6.56}$$

so that the true value $\phi(x_0, y_0) = x_0 y_0$ should lie within

$$\phi(\bar{x}, \bar{y}) \pm u_{\bar{\phi}}$$

$$u_{\bar{\phi}} = \frac{t_P(n-1)}{\sqrt{n}} \sqrt{\bar{y}^{\,2} s^2_x + 2\bar{x}\bar{y} s_{xy} + \bar{x}^{\,2} s^2_y} + (|\bar{y}| f_{s,x} + |\bar{x}| f_{s,y})\,. \tag{6.57}$$

Linearizing the quotient

$$\phi(x, y) = \frac{x}{y} \tag{6.58}$$

leads to

$$\phi(x_l, y_l) - \phi(\bar{x}, \bar{y}) = \frac{1}{\bar{y}}(x_l - \bar{x}) - \frac{\bar{x}}{\bar{y}^2}(y_l - \bar{y})\,; \quad l = 1, 2\,, \ldots,\, n\,.$$

Thus, the empirical variance follows from

$$s_\phi^2 = \frac{1}{\bar{y}^2}\, s_x^2 - 2\frac{\bar{x}}{\bar{y}^3}\, s_{xy} + \frac{\bar{x}^2}{\bar{y}^4}\, s_y^2 \,. \tag{6.59}$$

Considering the propagated systematic error

$$f_\phi = \frac{1}{\bar{y}} f_x + \frac{\bar{x}}{\bar{y}^2} f_y \,, \tag{6.60}$$

we have

$$\phi(\bar{x}, \bar{y}) \pm u_{\bar{\phi}} \tag{6.61}$$

$$u_{\bar{\phi}} = \frac{t_P(n-1)}{\sqrt{n}} \sqrt{\frac{1}{\bar{y}^2}\, s_x^2 - 2\frac{\bar{x}}{\bar{y}^3}\, s_{xy} + \frac{\bar{x}^2}{\bar{y}^4}\, s_y^2} + \left(\frac{1}{|\bar{y}|} f_{s,x} + \frac{|\bar{x}|}{|\bar{y}^2|} f_{s,y} \right) .$$

Given that X and Y are taken from standardized normal distributions, the random variable $U = X/Y$ follows a Cauchy density. Then, as is known, $E\{U\}$ and $E\{U^2\}$ would not exist. However, we confine ourselves to a non-pathological behavior of the quotient X/Y, so that the $\phi(x_l, y_l)$; $l = 1, \ldots, n$ as defined by the truncated Taylor series, may be considered to be (approximately) normally distributed.

Examples

We estimate the uncertainty of the conversion factor K_A, given the conversion factors $K_\mathrm{V} \pm u_{K_\mathrm{V}}$ and $K_\Omega \pm u_{K_\Omega}$. From

$$K_\mathrm{A} = \frac{K_\mathrm{V}}{K_\Omega}$$

we obtain

$$u_{K_\mathrm{A}} = \frac{t_P(n-1)}{\sqrt{n}} \sqrt{\frac{1}{K_\Omega^2}\, s_{K_\mathrm{V}}^2 - 2\frac{K_\mathrm{V}}{K_\Omega^3}\, s_{K_\mathrm{V}\, K_\Omega} + \frac{K_\mathrm{V}^2}{K_\Omega^4}\, s_{K_\Omega}^2}$$

$$+ \left(\frac{1}{K_\Omega} f_{s,K_\mathrm{V}} + \frac{K_\mathrm{V}}{K_\Omega^2} f_{s,K_\Omega} \right) .$$

We consider the Michelson–Morley experiment and estimate the uncertainty u_V of the displacement

$$V = 2L \left(\frac{u}{c} \right)^2$$

that the interference fringes should exhibit after 90° rotation of the interferometer. The quantity u denotes the Earth's velocity relative to the postulated ether, c the velocity of light and L the distance between any of the two all-silvered mirrors to the central half-silvered mirror. As $u/c \approx 10^{-4}$,

we observe $V \approx 2\,10^{-8}L$. Setting e.g. $L = 2 \times 10^7\,\lambda$ the displacement should be $V \approx 0.4\,\lambda$. Quite contrary to today's concepts, we naively consider c a measurand. Thus

$$u_V = \frac{t_P(n-1)}{\sqrt{n}}$$

$$\times \sqrt{\left(\frac{V}{L}\right)^2 s_L^2 + \left(\frac{2V}{u}\right)^2 s_u^2 + \left(\frac{2V}{c}\right)^2 s_c^2 + \frac{2V^2}{(Lu)} s_{Lu} - \frac{4V^2}{(uc)} s_{uc} - \frac{2V^2}{(Lc)} s_{Lc}}$$

$$+ \left[\left(\frac{V}{L}\right)_{s,L} + \left(\frac{2V}{u}\right) f_{s,u} + \left(\frac{2V}{c}\right) f_{s,c}\right] .$$

Though Michelson and Morley relied on a different approach to estimate the uncertainty of the displacement V, their result will endure.[3] This might willingly be taken as an opportunity to play down the importance of measurement uncertainties in general. Nevertheless, we are sure that scientific discoveries rely on vast fields of a priori knowledge, i.e. sound theoretical frameworks and decades of metrological experience as well as the understanding that any scientific concept has to be subjected to an all-decisive comparison between theory and experiment so that in the last analysis, it is the measurement uncertainty which is responsible for the result.

Comparisons will be particularly critical if experiments are operating close to the limits of verifiability and if their outgoings have far-reaching physical consequences – which applies, for example, to the still pending question of the correct neutrino model.

Simulation

As the true values of the measurands are unknown, there is no way to test a formalism estimating measurement uncertainties which relies on real, physically obtained data. Nevertheless, we are in a position to design numerical tests being based on simulated data, since under conditions of simulation, the true values are necessarily part of the model, and thus known a priori. We subject both formalisms, the one proposed here and that of the *ISO Guide*, to simulative tests. We "measure" the area of a rectangle whose side lengths are chosen to be $x_0 = 1\,\mathrm{cm}$ and $y_0 = 2\,\mathrm{cm}$, Fig. 6.2. In each case, we consider $n = 10$ repeat measurements for x and y respectively. Let the intervals limiting the systematic errors be

$$-10\,\mu\mathrm{m} \le f_x \le 10\,\mu\mathrm{m}\,, \quad -10\,\mu\mathrm{m} \le f_y \le 10\,\mu\mathrm{m}\,.$$

[3] The interpretation of the observation is as follows. If the arm of the interferometer lying parallel to the direction of motion of the Earth is shortened by a factor of $[1 - (u/c)^2]$, the displacement V vanishes numerically.

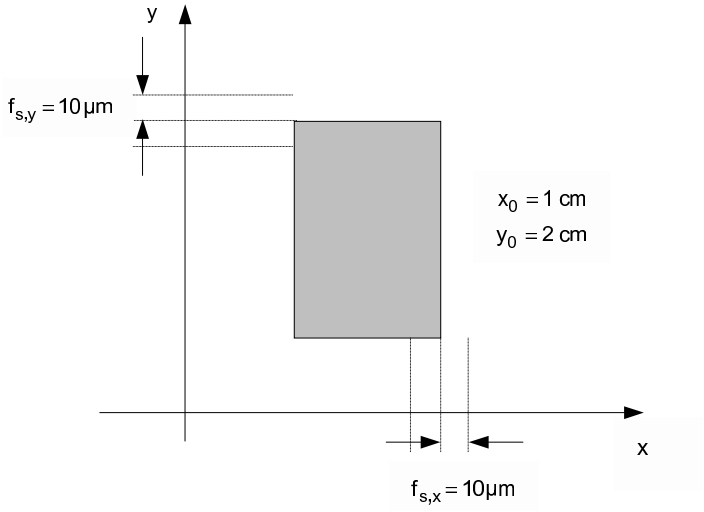


Fig. 6.2. Simulation of the measurement of the area of a rectangle

We adjust the variances σ_x^2, σ_y^2 of the simulated, normally distributed random errors to be equal to the postulated ISO variances of the systematic errors f_x, f_y,

$$\sigma_{f_x}^2 = \frac{f_{s,x}^2}{3} \quad \text{and} \quad \sigma_{f_y}^2 = \frac{f_{s,y}^2}{3}\,,$$

referring to rectangular densities over the two intervals given above.

According to the error model under discussion, the uncertainty $u_{\bar{x}\bar{y}}$ of the area $\bar{x}\bar{y}$ is given by

$$u_{\bar{x}\bar{y}} = \frac{t_P(n-1)}{\sqrt{n}} \sqrt{\bar{y}^{\,2} s_x^2 + 2\,\bar{x}\,\bar{y}\,s_{xy} + \bar{x}^{\,2} s_y^2} + |\bar{y}| f_{s,x} + |\bar{x}| f_{s,y} \qquad (6.62)$$

while the *ISO Guide* [36] would yield

$$u_{\bar{x}\bar{y}} = k_P \sqrt{\bar{y}^{\,2}\left[\frac{s_x^2}{n_x} + \frac{f_{s,x}^2}{3}\right] + \bar{x}^{\,2}\left[\frac{s_y^2}{n_y} + \frac{f_{s,y}^2}{3}\right]}\,. \qquad (6.63)$$

The error limits $f_{s,x} = 10\,\mu\text{m}$ and $f_{s,y} = 10\,\mu\text{m}$ enter (6.62) and (6.63). But, to simulate the "measuring data", we choose any values f_x, f_y from the pertaining intervals $\pm f_{s,x}$, $\pm f_{s,y}$ and superpose them on the simulated data. Let us consider some special cases. If f_x and f_y

- have different signs, we shall speak of error compensation,
- have the same sign, of error intensification,
- are permuted, of a test for symmetry.

As to ISO uncertainties, $k_P = 1$ is recommended for purposes of high-level metrology and $k_P = 2$ for standard cases. Within the alternative formalism we set $t_{68\%}(9) = 1.04$ and $t_{95\%}(9) = 2.26$, thus allowing meaningful comparisons.

Every "measurement" yields a result $\bar{x}\bar{y} \pm u_{\bar{x}\bar{y}}$. However, to arrive at statistically representative statements, we carry out 1000 complete cycles of measurements at a time, i.e. for any given choice of f_x = const. and f_y = const., we simulate 1000 new sets of random errors.

If $k_P = 1$, in the case of error intensification, the ISO model turns out to be unfit. Remarkably enough, the test for symmetry delivers only 59 positive results or successes, given that $f_x = 10\,\mu\text{m}$ and $f_y = 0\,\mu\text{m}$. However, if $f_x = 0\,\mu\text{m}$ and $f_y = 10\,\mu\text{m}$, we observe 841 successes. This observation is due to the disparity of the partial derivatives $\bar{y} \approx 2\,\text{cm}$ and $\bar{x} \approx 1\,\text{cm}$ which, in a sense, "weight" the errors.

The situation gets better on setting $k_P = 2$. This does not, however, apply to the most unfavorable case $f_x = f_y = 10\,\mu\text{m}$.

Clearly, as Tables 6.1 and 6.2 illustrate, occasionally used terms like "optimistically" or "pessimistically" estimated measurement uncertainties do not have any specific meaning. We neither give information away when quoting safe estimates nor regain information otherwise lost by keeping the measurement uncertainties tight. Measurement uncertainties should rather be simply objective.

Table 6.1. Localization of true values: *ISO Guide* versus alternative approach

1000 Simulations		$k_p = 1$		$t_{68\%}(9) = 1.04$	
in µm		ISO		alternative model	
f_x	f_y	successes	failures	successes	failures
compensation					
10	−10	815	185	1000	0
5	−5	986	14	1000	0
intensification					
10	10	0	1000	842	158
5	5	363	637	1000	0
symmetry					
10	0	59	941	1000	0
0	10	814	186	1000	0
5	0	796	204	1000	0
0	5	978	22	1000	0

6.5 Error Propagation over Several Stages

Even in experimentally simple situations, quantities to be linked up may present themselves as results of previous measurements and other functional relationships, so $\phi(x,y) = x/y$ could be a first and $\Gamma[y,\phi(x,y)] = y\exp[\phi(x,y)]$ a second combination. We consider the uncertainty $u_{\bar{\Gamma}}$, referring again to truncated series expansions and the notation $\bar{\Gamma} = \Gamma[\bar{y},\phi(\bar{x},\bar{y})]$.

Let us initially linearize $\phi(x,y)$,

$$\phi(x_l,y_l) = \phi(x_0,y_0) + \left[\frac{\partial\phi}{\partial\bar{x}}(x_l-\mu_x) + \frac{\partial\phi}{\partial\bar{y}}(y_l-\mu_y)\right] + \left[\frac{\partial\phi}{\partial\bar{x}}f_x + \frac{\partial\phi}{\partial\bar{y}}f_y\right],$$

$$\phi(\bar{x},\bar{y}) = \phi(x_0,y_0) + \left[\frac{\partial\phi}{\partial\bar{x}}(\bar{x}-\mu_x) + \frac{\partial\phi}{\partial\bar{y}}(\bar{y}-\mu_y)\right] + \left[\frac{\partial\phi}{\partial\bar{x}}f_x + \frac{\partial\phi}{\partial\bar{y}}f_y\right].$$

The expectation

$$\mu_\phi = \phi(x_0,y_0) + \frac{\partial\phi}{\partial\bar{x}}f_x + \frac{\partial\phi}{\partial\bar{y}}f_y \tag{6.64}$$

reveals a propagated systematic error of the kind

$$f_\phi = \frac{\partial\phi}{\partial\bar{x}}f_x + \frac{\partial\phi}{\partial\bar{y}}f_y\,. \tag{6.65}$$

We might wish to estimate f_ϕ as

Table 6.2. Localization of true values: *ISO Guide* versus alternative approach

1000 Simulations		$k_p = 2$		$t_{95\%}(9) = 2.26$	
in µm		ISO		alternative model	
f_x	f_y	successes	failures	successes	failures
compensation					
10	−10	1000	0	1000	0
5	−5	1000	0	1000	0
intensification					
10	10	232	768	974	26
5	5	999	1	1000	0
symmetry					
10	0	996	34	1000	0
0	10	1000	0	1000	0
5	0	1000	0	1000	0
0	5	1000	0	1000	0

$$-f_{s,\phi} \le f_\phi \le f_{s,\phi}\,, \quad f_{s,\phi} = \left|\frac{\partial\phi}{\partial\bar{x}}\right| f_{s,x} + \left|\frac{\partial\phi}{\partial\bar{y}}\right| f_{s,y} \tag{6.66}$$

which, however, should be postponed. Let us first refer to

$$\phi(x_l, y_l) - \phi(\bar{x}, \bar{y}) = \left[\frac{\partial\phi}{\partial\bar{x}}(x_l - \bar{x}) + \frac{\partial\phi}{\partial\bar{y}}(y_l - \bar{y})\right]. \tag{6.67}$$

Now, we expand $\Gamma[y, \phi(x, y)]$ twofold, abbreviating $\phi_l = \phi(x_l, y_l)$ and $\phi_0 = \phi(x_0, y_0)$,

$$\Gamma(y_l, \phi_l) = \Gamma(y_0, \phi_0) + \left[\frac{\partial\Gamma}{\partial\bar{y}}(y_l - \mu_x) + \frac{\partial\Gamma}{\partial\bar{\phi}}(\phi_l - \mu_\phi)\right] + \left[\frac{\partial\Gamma}{\partial\bar{y}} f_y + \frac{\partial\Gamma}{\partial\bar{\phi}} f_\phi\right],$$

$$\Gamma(\bar{y}, \bar{\phi}) = \Gamma(y_0, \phi_0) + \left[\frac{\partial\Gamma}{\partial\bar{y}}(\bar{y} - \mu_x) + \frac{\partial\Gamma}{\partial\bar{\phi}}(\bar{\phi} - \mu_\phi)\right] + \left[\frac{\partial\Gamma}{\partial\bar{y}} f_y + \frac{\partial\Gamma}{\partial\bar{\phi}} f_\phi\right].$$

This leads us to

$$\Gamma(y_l, \phi_l) - \Gamma(\bar{y}, \bar{\phi}) = \left[\frac{\partial\Gamma}{\partial\bar{y}}(y_l - \bar{y}) + \frac{\partial\Gamma}{\partial\bar{\phi}}(\phi_l - \bar{\phi})\right] \tag{6.68}$$

and

$$f_\Gamma = \left[\frac{\partial\Gamma}{\partial\bar{y}} f_y + \frac{\partial\Gamma}{\partial\bar{\phi}} f_\phi\right] \tag{6.69}$$

respectively. Finally, we insert (6.67) into (6.68),

$$\Gamma(y_l, \phi_l) - \Gamma(\bar{y}, \bar{\phi}) = \left[\frac{\partial\Gamma}{\partial\bar{\phi}}\frac{\partial\phi}{\partial\bar{x}}(x_l - \bar{x}) + \left(\frac{\partial\Gamma}{\partial\bar{y}} + \frac{\partial\Gamma}{\partial\bar{\phi}}\frac{\partial\phi}{\partial\bar{y}}\right)(y_l - \bar{y})\right] \tag{6.70}$$

and (6.65) into (6.69),

$$f_\Gamma = \frac{\partial\Gamma}{\partial\bar{\phi}}\frac{\partial\phi}{\partial\bar{x}} f_x + \left[\frac{\partial\Gamma}{\partial\bar{y}} + \frac{\partial\Gamma}{\partial\bar{\phi}}\frac{\partial\phi}{\partial\bar{y}}\right] f_y\,. \tag{6.71}$$

It is only now that we should estimate the propagated systematic error,

$$-f_{s,\Gamma} \le f_\Gamma \le f_{s,\Gamma}\,, \quad f_{s,\Gamma} = \left|\frac{\partial\Gamma}{\partial\bar{\phi}}\frac{\partial\phi}{\partial\bar{x}}\right| f_{s,x} + \left|\frac{\partial\Gamma}{\partial\bar{y}} + \frac{\partial\Gamma}{\partial\bar{\phi}}\frac{\partial\phi}{\partial\bar{y}}\right| f_{s,y}\,. \tag{6.72}$$

If, instead, we had subjected (6.69) to a worst case estimation

$$f^*_{s,\Gamma} = \left|\frac{\partial\Gamma}{\partial\bar{y}}\right| f_{s,y} + \left|\frac{\partial\Gamma}{\partial\bar{\phi}}\right| f_{s,\phi}$$

and had done the same with (6.65), we would have got

$$f^*_{s,\Gamma} = \left|\frac{\partial\Gamma}{\partial\bar{\phi}}\frac{\partial\phi}{\partial\bar{x}}\right| f_{s,x} + \left[\left|\frac{\partial\Gamma}{\partial\bar{y}}\right| + \left|\frac{\partial\Gamma}{\partial\bar{\phi}}\frac{\partial\phi}{\partial\bar{y}}\right|\right] f_{s,y}\,.$$

Obviously, this would be an inconsistent worst case estimation conflicting with the concepts of error propagation provided by the alternative error model. In other words, we had overlooked a dependency and, as a consequence, estimated too large a systematic error.

Referring to the abbreviations

$$b_x = \frac{\partial\Gamma}{\partial\bar{\phi}}\frac{\partial\phi}{\partial\bar{x}} \quad \text{and} \quad b_y = \frac{\partial\Gamma}{\partial\bar{y}} + \frac{\partial\Gamma}{\partial\bar{\phi}}\frac{\partial\phi}{\partial\bar{y}}$$

(6.70) and (6.71) yield

$$s^2_\Gamma = b^2_x s^2_x + 2b_x b_y s_{xy} + b^2_y s^2_y \tag{6.73}$$

and

$$f_\Gamma = b_x f_x + b_y f_y \tag{6.74}$$

respectively, so that

$$\Gamma(\bar{y},\bar{\phi}) \pm u_{\bar{\Gamma}} \tag{6.75}$$

$$u_{\bar{\Gamma}} = \frac{t_P(n-1)}{\sqrt{n}}\sqrt{b^2_x s^2_x + 2b_x b_y s_{xy} + b^2_y s^2_y} + [|b_x| f_{s,x} + |b_y| f_{s,y}]\,.$$

Just to prove the efficiency of this approach, we consider another relationship, namely

$$\Gamma\left[\phi(x, y\,, \ldots)\,, \psi(p, q\,, \ldots)\,, \ldots\right]\,.$$

Confining ourselves to two measurands, from

$$\Gamma(\phi_l, \psi_l) = \Gamma(\phi_0, \psi_0) + \frac{\partial\Gamma}{\partial\bar{\phi}}(\phi_l - \mu_\phi) + \frac{\partial\Gamma}{\partial\bar{\psi}}(\psi_l - \mu_\psi) + \frac{\partial\Gamma}{\partial\bar{\phi}} f_\phi + \frac{\partial\Gamma}{\partial\bar{\psi}} f_\psi$$

$$\Gamma(\bar{\phi},\bar{\psi}) = \Gamma(\phi_0, \psi_0) + \frac{\partial\Gamma}{\partial\bar{\phi}}(\bar{\phi} - \mu_\phi) + \frac{\partial\Gamma}{\partial\bar{\psi}}(\bar{\psi}_l - \mu_\psi) + \frac{\partial\Gamma}{\partial\bar{\phi}} f_\phi + \frac{\partial\Gamma}{\partial\bar{\psi}} f_\psi$$

we deduce

$$\Gamma(\phi_l, \psi_l) - \Gamma(\bar{\phi},\bar{\psi}) = \frac{\partial\Gamma}{\partial\bar{\phi}}(\phi_l - \bar{\phi}) + \frac{\partial\Gamma}{\partial\bar{\psi}}(\psi_l - \bar{\psi})\,,$$

and, furthermore,

$$f_\Gamma = \frac{\partial\Gamma}{\partial\bar{\phi}} f_\phi + \frac{\partial\Gamma}{\partial\bar{\psi}} f_\psi\,.$$

With

$$\phi_l - \bar{\phi} = \left[\frac{\partial\phi}{\partial\bar{x}}(x_l - \bar{x}) + \frac{\partial\phi}{\partial\bar{y}}(y_l - \bar{y})\right]; \quad f_\phi = \frac{\partial\phi}{\partial\bar{x}}f_x + \frac{\partial\phi}{\partial\bar{y}}f_y$$

$$\psi_l - \bar{\psi} = \left[\frac{\partial\psi}{\partial\bar{p}}(p_l - \bar{p}) + \frac{\partial\psi}{\partial\bar{q}}(q_l - \bar{q})\right]; \quad f_\psi = \frac{\partial\psi}{\partial\bar{p}}f_p + \frac{\partial\phi}{\partial\bar{q}}f_q$$

and

$$b_x = \frac{\partial\Gamma}{\partial\bar{\phi}}\frac{\partial\phi}{\partial\bar{x}}, \quad b_y = \frac{\partial\Gamma}{\partial\bar{\phi}}\frac{\partial\phi}{\partial\bar{y}}, \quad b_p = \frac{\partial\Gamma}{\partial\bar{\psi}}\frac{\partial\psi}{\partial\bar{p}}, \quad b_q = \frac{\partial\Gamma}{\partial\bar{\psi}}\frac{\partial\psi}{\partial\bar{q}}$$

we find

$$\Gamma(\phi_l, \psi_l) - \Gamma(\bar{\phi}, \bar{\psi}) = b_x(x_l - \bar{x}) + b_y(y_l - \bar{y}) + b_p(p_l - \bar{p}) + b_q(q_l - \bar{q})$$

and

$$f_\Gamma = b_x f_x + b_y f_y + b_p f_p + b_q f_q$$

respectively. Obviously, that part of the overall uncertainty $u_{\bar{\Gamma}}$ which is due to random errors includes the empirical covariances $s_{xy}, s_{xp}, s_{xq}, s_{yp}, s_{yq}, s_{pq}$, and this in turn means that the evaluation procedures rely on the original series of measurements, which, hopefully, will have been saved by the laboratories.

Part II

Least Squares Adjustment

7 Least Squares Formalism

7.1 Geometry of Adjustment

In a sense, the least squares adjustment of an inconsistent, overdetermined linear system relies on the idea of orthogonal projection. To illustrate this, let us consider a source emitting parallel light falling perpendicularly onto a screen. A rod held obliquely over the screen then casts a shadow, Fig. 7.1. This scenario may be considered to be an equivalent to the orthogonal projection of the method of least squares.

Let us develop this idea to solve the following problem. Given n repeat measurements

$$x_1, x_2, \ldots, x_n\,,$$

how can we find an estimator $\bar{\beta}$ for the unknown true value x_0? Referring n times to the error equations (2.3), we are faced with

$$\begin{array}{ccccccc} x_1 & = & x_0 & + & \varepsilon_1 & + & f \\ x_2 & = & x_0 & + & \varepsilon_2 & + & f \\ \multicolumn{7}{c}{\dots\dots\dots\dots\dots\dots\dots} \\ x_n & = & x_0 & + & \varepsilon_n & + & f\,. \end{array} \tag{7.1}$$

By means of an auxiliary vector

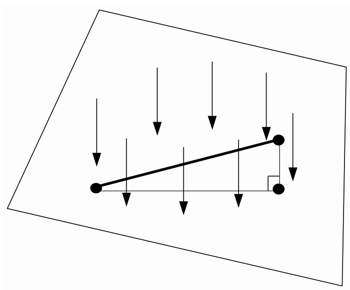


Fig. 7.1. The method of least squares, presented as an orthogonal projection of a rod, held obliquely over a screen

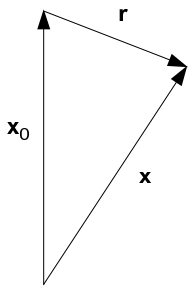


Fig. 7.2. Vector $\boldsymbol{x}$ of input data, vector $\boldsymbol{r}$ of residuals and true solution vector $\boldsymbol{x}_0$

$$\boldsymbol{a} = (1 \quad 1 \quad \cdots \quad 1)^{\mathrm{T}} ,$$

we may formally define a true solution vector $\boldsymbol{x}_0 = \boldsymbol{a}x_0$. Putting

$$\boldsymbol{x} = (x_1 \quad x_2 \quad \cdots \quad x_n)^{\mathrm{T}} \quad \text{and} \quad \boldsymbol{\varepsilon} = (\varepsilon_1 \quad \varepsilon_2 \quad \cdots \quad \varepsilon_n)^{\mathrm{T}}$$

(7.1) takes the form

$$\boldsymbol{x} = \boldsymbol{x}_0 + \boldsymbol{\varepsilon} + \boldsymbol{f} .$$

As $\bar{\beta}$ is unknown, we introduce a variable β instead:

$$\beta \approx x_1 , \quad \beta \approx x_2 , \quad \ldots , \quad \beta \approx x_n ,$$

or, in vector form,

$$\begin{pmatrix} 1 \\ 1 \\ \cdots \\ 1 \end{pmatrix} \beta \approx \begin{pmatrix} x_1 \\ x_2 \\ \cdots \\ x_n \end{pmatrix} , \quad \text{i.e.} \quad \boldsymbol{a}\beta \approx \boldsymbol{x} . \tag{7.2}$$

If $\boldsymbol{x}$ had no errors, we would have $\boldsymbol{a}\beta_0 = \boldsymbol{x}_0$, i.e. $\beta_0 = x_0$. In a sense, we may understand the vector $\boldsymbol{a}$ to span a one-dimensional space holding the true solution vector $\boldsymbol{x_0}$.

As there are measurement errors, we purposefully quantify the discrepancy between $\boldsymbol{x}$ and $\boldsymbol{x}_0$ by the vector

$$\boldsymbol{r} = \boldsymbol{x} - \boldsymbol{x}_0 ,$$

the components of which are called residuals, Fig. 7.2. As the vector space $\boldsymbol{a}$ holds the true solution vector $\boldsymbol{x}_0$, we assume that just this space will hold the approximation to (7.2) we are looking for. Indeed, the method of least squares "solves" the inconsistent system (7.2) by orthogonally projecting $\boldsymbol{x}$ onto $\boldsymbol{a}||\boldsymbol{x}_0$. With $\boldsymbol{P}$ denoting the appropriate projection operator, we have

$$\boldsymbol{a}\bar{\beta} = \boldsymbol{P}\boldsymbol{x} . \tag{7.3}$$

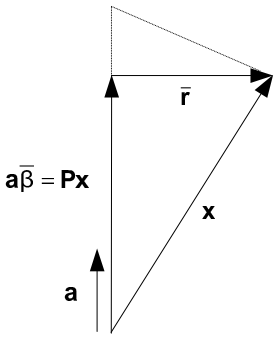


Fig. 7.3. Orthogonal projection $\boldsymbol{Px}$ of $\boldsymbol{x}$ onto $\boldsymbol{a}$; $\bar{\boldsymbol{r}}$ vector of residuals of minimal length; $\bar{\beta}$ stretch factor

The stretch factor $\bar{\beta}$ by which $\boldsymbol{a}$ has to be multiplied so that (7.3) is fulfilled is considered to be the least squares estimator of the inconsistent system (7.2). Figure 7.3 illustrates the proposal. We prove:

The orthogonal projection of $\boldsymbol{x}$ *onto* $\boldsymbol{a}$ *minimizes the Euclidean norm of* $\boldsymbol{r}$.

To this end, an arbitrary vector of residuals $\boldsymbol{r} = \boldsymbol{x} - \boldsymbol{a}\beta$ is likened with the vector of residuals being due to the orthogonal projection,

$$\bar{\boldsymbol{r}} = \boldsymbol{x} - \boldsymbol{a}\bar{\beta}\,.$$

The identity

$$\boldsymbol{r} = \boldsymbol{x} - \boldsymbol{a}\beta = (\boldsymbol{x} - \boldsymbol{a}\bar{\beta}) + \boldsymbol{a}(\bar{\beta} - \beta)$$

yields

$$\boldsymbol{r}^{\mathrm{T}}\boldsymbol{r} = \bar{\boldsymbol{r}}^{\mathrm{T}}\bar{\boldsymbol{r}} + \boldsymbol{a}^{\mathrm{T}}\boldsymbol{a}(\bar{\beta} - \beta)^2\,,$$

i.e.

$$\boldsymbol{r}^{\mathrm{T}}\boldsymbol{r} \geq \bar{\boldsymbol{r}}^{\mathrm{T}}\bar{\boldsymbol{r}}\,.$$

Usually, this result is established by differentiating an expression of the form

$$Q = (x_1 - \beta)^2 + (x_2 - \beta)^2 + \cdots + (x_n - \beta)^2$$

with respect to β. This sum, called the sum of squared residuals, is obviously established by squaring and summing up the components of the vector $\boldsymbol{r} = \boldsymbol{x} - \boldsymbol{a}\beta$. However, here we prefer to trace the method of least squares back to the idea of orthogonal projections. From

$$\boldsymbol{a}^{\mathrm{T}}\bar{\boldsymbol{r}} = \boldsymbol{a}^{\mathrm{T}}(\boldsymbol{x} - \boldsymbol{a}\bar{\beta}) = 0\,, \quad \text{i.e.} \quad \boldsymbol{a}^{\mathrm{T}}\boldsymbol{a}\,\bar{\beta} = \boldsymbol{a}^{\mathrm{T}}\boldsymbol{x} \tag{7.4}$$

we infer

$$\bar{\beta} = (\boldsymbol{a}^{\mathrm{T}}\boldsymbol{a})^{-1}\boldsymbol{a}^{\mathrm{T}}\boldsymbol{x}\,. \tag{7.5}$$

Hence, in this introductory example, the required least squares estimator is nothing but the arithmetic mean

$$\bar{\beta} = \frac{1}{n}\sum_{l=1}^{n} x_l$$

of n observations x_l; $l = 1, \ldots, n$. Let us summarize: $\boldsymbol{a}$ and $\boldsymbol{x}$ are vectors of an n-dimensional space. The orthogonal projection of $\boldsymbol{x}$, presented in (7.3), onto a one-dimensional space, spanned by $\boldsymbol{a}$, has produced the stretch factor or estimator $\bar{\beta} = \bar{x}$. Thus, the orthogonal projection has "solved" the inconsistent system (7.2) in terms of least squares.

To find the projection operator $\boldsymbol{P}$, we multiply $\boldsymbol{a}^{\mathrm{T}}\boldsymbol{a}\bar{\beta} = \boldsymbol{a}^{\mathrm{T}}\boldsymbol{x}$ on the left by $\boldsymbol{a}(\boldsymbol{a}^{\mathrm{T}}\boldsymbol{a})^{-1}$,

$$\boldsymbol{a}\,\bar{\beta} = \boldsymbol{a}(\boldsymbol{a}^{\mathrm{T}}\boldsymbol{a})^{-1}\boldsymbol{a}^{\mathrm{T}}\boldsymbol{x}\,,$$

so that

$$\boldsymbol{P} = \boldsymbol{a}(\boldsymbol{a}^{\mathrm{T}}\boldsymbol{a})^{-1}\boldsymbol{a}^{\mathrm{T}}\,. \tag{7.6}$$

In this particular case, all elements of $\boldsymbol{P}$ exhibit the same value $1/n$. Multiplying (7.3) on the left by $\boldsymbol{a}^{\mathrm{T}}$ yields

$$\boldsymbol{a}^{\mathrm{T}}\boldsymbol{a}\bar{\beta} = \boldsymbol{a}^{\mathrm{T}}\boldsymbol{P}\boldsymbol{x} = \boldsymbol{a}^{\mathrm{T}}\boldsymbol{x}\,, \quad \text{i.e.} \quad \bar{\beta} = (\boldsymbol{a}^{\mathrm{T}}\boldsymbol{a})^{-1}\boldsymbol{a}^{\mathrm{T}}\boldsymbol{x}\,.$$

The method of least squares cannot do wonders: all it can do is to transfer the approximation

$$\boldsymbol{a}\beta \approx \boldsymbol{x}\,,$$

say by means of a gimmick, into a formally self-consistent statement, namely

$$\boldsymbol{a}\bar{\beta} = \boldsymbol{P}\boldsymbol{x}\,.$$

The input data need not fulfil any presumptions at all. The orthogonal projection "adjusts" any kind of contradiction in like manner, so that fatal errors of reasoning and the finest, metrologically unavoidable, errors of measurement are treated side by side on the same level.

The vector of residuals, $\bar{\boldsymbol{r}} = \boldsymbol{x} - \boldsymbol{a}\bar{\beta}$, is in no way related to physical errors. As $\bar{\boldsymbol{r}}$ is due to an orthogonal projection, its components are mathematically defined auxiliary quantities. However, the components of the vector $\boldsymbol{r} = \boldsymbol{x} - \boldsymbol{x}_0$ are physically meaningful error sums.

7.2 Unconstrained Adjustment

Let us assume that the measuring problem has led us to a set of linear relationships

$$\begin{array}{ccccccccc} a_{11}\beta_1 & + & a_{12}\beta_2 & + & \cdots & + & a_{1r}\beta_r & = & x_1 \\ a_{21}\beta_1 & + & a_{22}\beta_2 & + & \cdots & + & a_{2r}\beta_r & = & x_2 \\ \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots \\ a_{m1}\beta_1 & + & a_{m2}\beta_2 & + & \cdots & + & a_{mr}\beta_r & = & x_m\,. \end{array} \tag{7.7}$$

To cast this in matrix notation, we introduce an $(m \times r)$ matrix $\boldsymbol{A}$ of coefficients a_{ik}, an $(m \times 1)$ column vector $\boldsymbol{x}$, assembling the right-hand sides x_i, and finally, an $(r \times 1)$ column vector $\boldsymbol{\beta}$ of unknowns β_k. From

$$\boldsymbol{A} = \begin{pmatrix} a_{11} & a_{12} & \dots & a_{1r} \\ a_{21} & a_{22} & \dots & a_{2r} \\ \dots & \dots & \dots & \dots \\ a_{m1} & a_{m2} & \dots & a_{mr} \end{pmatrix}, \quad \boldsymbol{x} = \begin{pmatrix} x_1 \\ x_2 \\ \dots \\ x_m \end{pmatrix}, \quad \boldsymbol{\beta} = \begin{pmatrix} \beta_1 \\ \beta_2 \\ \dots \\ \beta_r \end{pmatrix}$$

we find

$$\boldsymbol{A\beta} = \boldsymbol{x}\,.$$

This system is solvable if and only if the vector $\boldsymbol{x}$ may be expressed as a linear combination of the column vectors of $\boldsymbol{A}$,

$$\boldsymbol{a}_k = \begin{pmatrix} a_{1k} \\ a_{2k} \\ \dots \\ a_{mk} \end{pmatrix}; \quad k = 1, \dots, r\,,$$

so that

$$\beta_1 \begin{pmatrix} a_{11} \\ a_{21} \\ \dots \\ a_{m1} \end{pmatrix} + \beta_2 \begin{pmatrix} a_{12} \\ a_{22} \\ \dots \\ a_{m2} \end{pmatrix} + \cdots + \beta_r \begin{pmatrix} a_{1r} \\ a_{2r} \\ \dots \\ a_{mr} \end{pmatrix} = \boldsymbol{x}\,.$$

If this applies, $\boldsymbol{x}$ is inside the column space of $\boldsymbol{A}$; if not, the linear system is inconsistent or algebraically unsolvable.

Any experimental implementation of relationships (7.7), being conceptually exact, entails measurement errors so that

$$\boldsymbol{A\beta} \approx \boldsymbol{x} \tag{7.8}$$

which means that $\boldsymbol{x}$ is outside the column space of $\boldsymbol{A}$. To quantify the discrepancy, we again refer to a vector $\boldsymbol{r}$ of residuals,

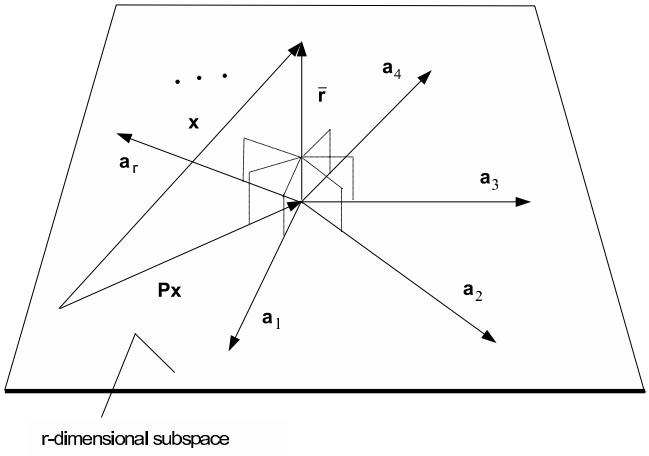


Fig. 7.4. The vector $\bar{\boldsymbol{r}}$ of residuals is perpendicular to the r-dimensional subspace, spanned by the column vectors $\boldsymbol{a_k}$; $k = 1, \ldots, r$

$$\boldsymbol{r} = \boldsymbol{x} - \boldsymbol{A}\boldsymbol{\beta}\,.$$

As has been discussed, we require the solution vector $\bar{\boldsymbol{\beta}}$ to minimize the sum of squared residuals.

In the following, we assume

$$m > r \quad \text{and} \quad \operatorname{rank}(\boldsymbol{A}) = r$$

The vectors $\boldsymbol{a}_k$; $k = 1, \ldots, r$ define an r-dimensional subspace of an m-dimensional space. Of course, $\boldsymbol{x}$ is an element of the latter, however, on account of measurement errors, not an element of the former. By means of a projection operator $\boldsymbol{P}$ the method of least squares throws $\boldsymbol{x}$ orthogonally onto the subspace spanned by the r column vectors $\boldsymbol{a}_k$ and substitutes the projection $\boldsymbol{P}\boldsymbol{x}$ for the erroneous vector $\boldsymbol{x}$ so that, as shown in Fig. 7.4,

$$\boldsymbol{A}\bar{\boldsymbol{\beta}} = \boldsymbol{P}\boldsymbol{x}\,. \tag{7.9}$$

Obviously, the vector $\boldsymbol{P}\boldsymbol{x}$ so defined is a linear combination of the column vectors $\boldsymbol{a}_k$. Hence, (7.9) is self-consistent and solvable. Its solution vector $\bar{\boldsymbol{\beta}}$ solves (7.8) in terms of least squares. The components $\bar{\beta}_k$; $k = 1, \ldots, r$ of $\bar{\boldsymbol{\beta}}$ may be seen to stretch the column vectors $\boldsymbol{a}_k$ of $\boldsymbol{A}$, rendering (7.9) possible.

Due to the orthogonality of the projection of $\boldsymbol{x}$, the vector of residuals

$$\bar{\boldsymbol{r}} = \boldsymbol{x} - \boldsymbol{A}\bar{\boldsymbol{\beta}} \tag{7.10}$$

is perpendicular to each of the column vectors of $\boldsymbol{A}$,

$$\boldsymbol{A}^{\mathrm{T}}\bar{\boldsymbol{r}} = \boldsymbol{0}\,.$$

Inserting (7.10), we obtain

$$\boldsymbol{A}^{\mathrm{T}}\boldsymbol{A}\bar{\boldsymbol{\beta}} = \boldsymbol{A}^{\mathrm{T}}\boldsymbol{x}\,,$$

so that

$$\bar{\boldsymbol{\beta}} = \boldsymbol{B}^{\mathrm{T}}\boldsymbol{x}\,, \tag{7.11}$$

where, to abbreviate,

$$\boldsymbol{B} = \boldsymbol{A}(\boldsymbol{A}^{\mathrm{T}}\boldsymbol{A})^{-1} \tag{7.12}$$

has been set. The definition of projection operators is independent of the method of least squares, see Appendix D. For now we are content with a heuristic derivation of $\boldsymbol{P}$. Multiplying $\boldsymbol{A}^{\mathrm{T}}\boldsymbol{A}\bar{\boldsymbol{\beta}} = \boldsymbol{A}^{\mathrm{T}}\boldsymbol{x}$ on the left by $\boldsymbol{B}$ yields $\boldsymbol{A}\bar{\boldsymbol{\beta}} = \boldsymbol{A}(\boldsymbol{A}^{\mathrm{T}}\boldsymbol{A})^{-1}\boldsymbol{A}^{\mathrm{T}}\boldsymbol{x}$, i.e.

$$\boldsymbol{P} = \boldsymbol{A}(\boldsymbol{A}^{\mathrm{T}}\boldsymbol{A})^{-1}\boldsymbol{A}^{\mathrm{T}}\,. \tag{7.13}$$

By means of the identity

$$\boldsymbol{r} = \boldsymbol{x} - \boldsymbol{A}\boldsymbol{\beta} = (\boldsymbol{x} - \boldsymbol{A}\bar{\boldsymbol{\beta}}) + \boldsymbol{A}(\bar{\boldsymbol{\beta}} - \boldsymbol{\beta})$$

we again prove that the Euclidean norm

$$\boldsymbol{r}^{\mathrm{T}}\boldsymbol{r} = \bar{\boldsymbol{r}}^{\mathrm{T}}\bar{\boldsymbol{r}} + (\bar{\boldsymbol{\beta}} - \boldsymbol{\beta})^{\mathrm{T}}\boldsymbol{A}^{\mathrm{T}}\boldsymbol{A}(\bar{\boldsymbol{\beta}} - \boldsymbol{\beta})$$

of any vector of residuals $\boldsymbol{r} = \boldsymbol{x} - \boldsymbol{A}\boldsymbol{\beta}$ can never be smaller than the Euclidean norm of the vector of residuals $\bar{\boldsymbol{r}}$ resulting from the orthogonal projection, i.e.

$$\boldsymbol{r}^{\mathrm{T}}\boldsymbol{r} \geq \bar{\boldsymbol{r}}^{\mathrm{T}}\bar{\boldsymbol{r}}\,.$$

The product $\boldsymbol{A}^{\mathrm{T}}\boldsymbol{A}$ is invertible if the column vectors of the design matrix $\boldsymbol{A}$ are independent, i.e. if $\boldsymbol{A}$ has rank r, see Appendix A.

Uncertainty assignments ask for well-defined reference values. Consequently, for any empirical input vectors $\boldsymbol{x}$ obtained metrologically, we have to introduce a true vector $\boldsymbol{x}_0$ the components $x_{0,i}$ of which are the true values of the measurands x_i,

$$\boldsymbol{x}_0 = (x_{0,1} \quad x_{0,2} \quad \cdots \quad x_{0,m})^{\mathrm{T}}\,.$$

If $\boldsymbol{x}_0$ was known, r equations would be sufficient to determine the r unknown components $\beta_{0,k}$ of the true solution vector $\boldsymbol{\beta}_0$. But assuming the linear system to be both physically and mathematically well defined, we may nevertheless deduce $\boldsymbol{\beta}_0$ referring to all $m > r$ equations,

$$\boldsymbol{\beta}_0 = (\boldsymbol{A}^{\mathrm{T}}\boldsymbol{A})^{-1}\boldsymbol{A}^{\mathrm{T}}\boldsymbol{x}_0\,.$$

As $\boldsymbol{A}$ is rectangular, an inverse is not defined. However, we may take $(\boldsymbol{A}^{\mathrm{T}}\boldsymbol{A})^{-1}\boldsymbol{A}^{\mathrm{T}}$ as a pseudo-inverse.

7.3 Constrained Adjustment

We demand the least-squares solution vector $\bar{\boldsymbol{\beta}}$ of the overdetermined, inconsistent linear system

$$\boldsymbol{A}\boldsymbol{\beta} \approx \boldsymbol{x} \tag{7.14}$$

not only to reconcile the linear system with the measurement errors of the input data, but to also consistently comply with a given set of linear constraints of the form

$$\boldsymbol{H}\boldsymbol{\beta} = \boldsymbol{y}\,, \tag{7.15}$$

where $\boldsymbol{H}$ is an $(q \times r)$ matrix of rank q. The least squares vector $\bar{\boldsymbol{\beta}}$ is required to satisfy $\boldsymbol{H}\bar{\boldsymbol{\beta}} = \boldsymbol{y}$. The problem solving procedure depends on the rank of the system matrix $\boldsymbol{A}$. Initially, we assume

$$\operatorname{rank}(\boldsymbol{A}) = r\,.$$

Certainly, the projection operator $\boldsymbol{P} = \boldsymbol{A}(\boldsymbol{A}^{\mathrm{T}}\boldsymbol{A})^{-1}\boldsymbol{A}^{\mathrm{T}}$ used until now would produce a vector $\bar{\boldsymbol{\beta}}$ that is incompatible with the constraints. Consequently, we have to modify the quiddity of the orthogonal projection. Indeed, as will be shown in Appendix E, a projection operator of the form

$$\boldsymbol{P} = \boldsymbol{A}(\boldsymbol{A}^{\mathrm{T}}\boldsymbol{A})^{-1}\boldsymbol{A}^{\mathrm{T}} - \boldsymbol{C}(\boldsymbol{C}^{\mathrm{T}}\boldsymbol{C})^{-1}\boldsymbol{C}^{\mathrm{T}}$$

meets the purpose. The least squares solution vector is

$$\begin{aligned}\bar{\boldsymbol{\beta}} = {} & (\boldsymbol{A}^{\mathrm{T}}\boldsymbol{A})^{-1}\boldsymbol{A}^{\mathrm{T}}\boldsymbol{x} - (\boldsymbol{A}^{\mathrm{T}}\boldsymbol{A})^{-1}\boldsymbol{H}^{\mathrm{T}}\left[\boldsymbol{H}(\boldsymbol{A}^{\mathrm{T}}\boldsymbol{A})^{-1}\boldsymbol{H}^{\mathrm{T}}\right]^{-1} \\ & \times \left[\boldsymbol{H}(\boldsymbol{A}^{\mathrm{T}}\boldsymbol{A})^{-1}\boldsymbol{A}^{\mathrm{T}}\boldsymbol{x} - \boldsymbol{y}\right]\end{aligned} \tag{7.16}$$

fulfilling exactly $\boldsymbol{H}\bar{\boldsymbol{\beta}} = \boldsymbol{y}$. Now consider

$$\operatorname{rank}(\boldsymbol{A}) = r' < r\,.$$

We add $q = r - r'$ constraints

$$\boldsymbol{H}\boldsymbol{\beta} = \boldsymbol{y}\,, \tag{7.17}$$

where $\operatorname{rank}(\boldsymbol{H}) = q$, and combine the two systems (7.14) and (7.17). Though the product $\boldsymbol{A}^{\mathrm{T}}\boldsymbol{A}$ is not invertible, the sum of products $\boldsymbol{A}^{\mathrm{T}}\boldsymbol{A} + \boldsymbol{H}^{\mathrm{T}}\boldsymbol{H}$ is. The least squares solution vector turns out as

$$\bar{\boldsymbol{\beta}} = (\boldsymbol{A}^{\mathrm{T}}\boldsymbol{A} + \boldsymbol{H}^{\mathrm{T}}\boldsymbol{H})^{-1}(\boldsymbol{A}^{\mathrm{T}}\boldsymbol{x} + \boldsymbol{H}^{\mathrm{T}}\boldsymbol{y})\,, \tag{7.18}$$

satisfying $\boldsymbol{H}\bar{\boldsymbol{\beta}} = \boldsymbol{y}$.

8 Consequences of Systematic Errors

8.1 Structure of the Solution Vector

In the following we shall confine ourselves to unconstrained adjustments, i.e. to linear systems of the kind (7.8),

$$\boldsymbol{A}\boldsymbol{\beta} \approx \boldsymbol{x}\,. \tag{8.1}$$

With respect to the assessment of uncertainties, constrained adjustments would not introduce new aspects. As a matter of principle, any vector $\boldsymbol{x}$ of input data could be subjected to a least squares adjustment, given the matrix $\boldsymbol{A}$ has full rank and there is a true vector $\boldsymbol{x}_0$ underlying the erroneous input data, i.e. if alongside (8.1) there is a consistent system of the form

$$\boldsymbol{A}\boldsymbol{\beta}_0 = \boldsymbol{x}_0\,.$$

While the geometry of the least squares adjustment distinguishes the errors of the input data neither with respect to their causes nor with respect to their properties, as it is but an orthogonal projection, the situation gets different when we intend to estimate measurement uncertainties.

The column vector

$$\boldsymbol{x} = (x_1 \quad x_2 \quad \cdots \quad x_m)^{\mathrm{T}}$$

contains m erroneous input data

$$x_i = x_{0,i} + (x_i - \mu_i) + f_i\,; \quad i = 1, \ldots, m\,. \tag{8.2}$$

The $x_{0,i}$ denote the true values of the observations x_i, the differences $(x_i - \mu_i)$ their random errors ε_i and, finally, the f_i systematic errors which we consider to be constant in time. Further, we assume the ε_i to be independent and normally distributed. At present we shall abstain from repeat measurements.

The expected values of the random variables X_i; $i = 1, \ldots, m$ are given by

$$\mu_i = E\{X_i\} = x_{0,i} + f_i\,; \quad i = 1, \ldots, m\,. \tag{8.3}$$

Converting (8.2) into vector form yields

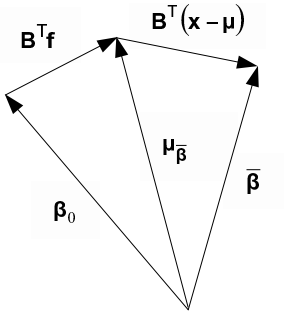


Fig. 8.1. The least squares solution vector $\bar{\boldsymbol{\beta}}$ is given by the sum of the true solution vector $\boldsymbol{\beta}_0$ and the vectors $\boldsymbol{B}^{\mathrm{T}}(\boldsymbol{x}-\boldsymbol{\mu})$ and $\boldsymbol{B}^{\mathrm{T}}\boldsymbol{f}$ being due to random and systematic errors respectively

$$\boldsymbol{x} = \begin{pmatrix} x_1 \\ x_2 \\ \cdots \\ x_m \end{pmatrix} = \begin{pmatrix} x_{0,1} \\ x_{0,2} \\ \cdots \\ x_{0,m} \end{pmatrix} + \begin{pmatrix} x_1 - \mu_1 \\ x_2 - \mu_2 \\ \cdots \\ x_m - \mu_m \end{pmatrix} + \begin{pmatrix} f_1 \\ f_2 \\ \cdots \\ f_m \end{pmatrix}$$

or

$$\boldsymbol{x} = \boldsymbol{x}_0 + (\boldsymbol{x}-\boldsymbol{\mu}) + \boldsymbol{f}\,. \tag{8.4}$$

We now decompose the least squares solution vector

$$\bar{\boldsymbol{\beta}} = \left(\boldsymbol{A}^{\mathrm{T}}\boldsymbol{A}\right)^{-1}\boldsymbol{A}^{\mathrm{T}}\boldsymbol{x} = \boldsymbol{B}^{\mathrm{T}}\boldsymbol{x}\,; \quad \boldsymbol{B} = \boldsymbol{A}\left(\boldsymbol{A}^{\mathrm{T}}\boldsymbol{A}\right)^{-1} \tag{8.5}$$

into

$$\bar{\boldsymbol{\beta}} = \boldsymbol{B}^{\mathrm{T}}\left[\boldsymbol{x}_0 + (\boldsymbol{x}-\boldsymbol{\mu}) + \boldsymbol{f}\right] = \boldsymbol{\beta}_0 + \boldsymbol{B}^{\mathrm{T}}(\boldsymbol{x}-\boldsymbol{\mu}) + \boldsymbol{B}^{\mathrm{T}}\boldsymbol{f}\,. \tag{8.6}$$

Obviously,

$$\boldsymbol{\beta}_0 = \left(\boldsymbol{A}^{\mathrm{T}}\boldsymbol{A}\right)^{-1}\boldsymbol{A}^{\mathrm{T}}\boldsymbol{x}_0 = \boldsymbol{B}^{\mathrm{T}}\boldsymbol{x}_0 \tag{8.7}$$

designates the true solution vector. As (8.6) and Fig. 8.1 underscore, the least squares estimator $\bar{\boldsymbol{\beta}}$ is given by the sum of the true solution vector $\boldsymbol{\beta}_0$ and two further terms $\boldsymbol{B}^{\mathrm{T}}(\boldsymbol{x}-\boldsymbol{\mu})$ and $\boldsymbol{B}^{\mathrm{T}}\boldsymbol{f}$ expressing the propagation of random and systematic errors respectively.

Within the framework of the concept of a statistical ensemble of measuring devices biased by one and the same systematic error, the estimator $\bar{\boldsymbol{\beta}}$ scatters with respect to the expectation

$$\boldsymbol{\mu}_{\bar{\boldsymbol{\beta}}} = E\left\{\bar{\boldsymbol{\beta}}\right\} = \boldsymbol{\beta}_0 + \boldsymbol{B}^{\mathrm{T}}\boldsymbol{f} \tag{8.8}$$

and not with respect to the true solution vector $\boldsymbol{\beta}_0$. On this note, we propose:

Given the input data are charged by unknown systematic errors, the least squares solution vector $\bar{\boldsymbol{\beta}}$ is biased with respect to the true solution vector $\boldsymbol{\beta}_0$.

Just this bias rules out most of the classical least squares tools.

8.2 Minimized Sum of Squared Residuals

Systematic errors provide the minimized sum of squared residuals with new properties.

For simplicity, we assume the random errors $\varepsilon_i = x_i - \mu_i$ to relate to the same parent distribution. We then have

$$\sigma^2 = E\left\{(X_i - \mu_i)^2\right\}\ ; \quad i = 1, \ldots, m\,. \tag{8.9}$$

If the input data were free from systematic errors, the unweighted minimized sum of squared residuals

$$\bar{Q}_{\text{unweighted}} = \bar{\boldsymbol{r}}^{\mathrm{T}}\bar{\boldsymbol{r}} = \left(\boldsymbol{x} - \boldsymbol{A}\bar{\boldsymbol{\beta}}\right)^{\mathrm{T}}\left(\boldsymbol{x} - \boldsymbol{A}\bar{\boldsymbol{\beta}}\right) \tag{8.10}$$

would supply an estimator for (8.9), namely

$$s^2 = \frac{\bar{Q}_{\text{unweighted}}}{m - r} \approx \sigma^2\,. \tag{8.11}$$

Considering (8.4), (7.10) and (7.13),

$$\begin{aligned}\bar{\boldsymbol{r}} &= \boldsymbol{x} - \boldsymbol{A}\bar{\boldsymbol{\beta}} = \boldsymbol{x} - \boldsymbol{P}\boldsymbol{x} \\ &= \boldsymbol{x}_0 + (\boldsymbol{x} - \boldsymbol{\mu}) + \boldsymbol{f} - \boldsymbol{P}\left[\boldsymbol{x}_0 + (\boldsymbol{x} - \boldsymbol{\mu}) + \boldsymbol{f}\right] \\ &= (\boldsymbol{x} - \boldsymbol{\mu}) - \boldsymbol{P}\,(\boldsymbol{x} - \boldsymbol{\mu}) + (\boldsymbol{f} - \boldsymbol{P}\boldsymbol{f})\ ,\end{aligned} \tag{8.12}$$

and temporarily ignoring the last term $(\boldsymbol{f} - \boldsymbol{P}\boldsymbol{f})$ on the right-hand side, we find

$$\bar{Q}_{\text{unweighted}} = (\boldsymbol{x} - \boldsymbol{\mu})^{\mathrm{T}}\,(\boldsymbol{I} - \boldsymbol{P})\,(\boldsymbol{x} - \boldsymbol{\mu})\ .$$

Here $\boldsymbol{I}$ denotes an $(m \times m)$ identity matrix. Dividing by σ^2 produces the weighted sum of squared residuals

$$\bar{Q}_{\text{weighted}} = \frac{(\boldsymbol{x} - \boldsymbol{\mu})^{\mathrm{T}}}{\sigma}\,(\boldsymbol{I} - \boldsymbol{P})\,\frac{(\boldsymbol{x} - \boldsymbol{\mu})}{\sigma}\,. \tag{8.13}$$

We shall show that $\bar{Q}_{\text{weighted}}$ is χ^2-distributed with $m - r$ degrees of freedom.

The matrices $\boldsymbol{I}, \boldsymbol{P}$ and $\boldsymbol{I} - \boldsymbol{P}$ are projection matrices, see Appendix D. As $\text{rank}(\boldsymbol{I} - \boldsymbol{P}) = m - r$, the difference matrix $\boldsymbol{I} - \boldsymbol{P}$ has $m - r$ non-zero eigenvalues, all having the same value 1. The remaining r eigenvalues are zero.

Let $\boldsymbol{T}$ denote an orthogonal $(m \times m)$ matrix and $\boldsymbol{I}$ an $(m \times m)$ identity matrix so that $\boldsymbol{T}^{\mathrm{T}}\boldsymbol{T} = \boldsymbol{T}\,\boldsymbol{T}^{\mathrm{T}} = \boldsymbol{I}$, $\boldsymbol{T}^{\mathrm{T}} = \boldsymbol{T}^{-1}$. Following the *spectral theorem of algebra* [52], we put the orthogonal eigenvectors of $\boldsymbol{I} - \boldsymbol{P}$ into the columns of $\boldsymbol{T}$ so that

$$\boldsymbol{T}^{\mathrm{T}}(\boldsymbol{I}-\boldsymbol{P})\boldsymbol{T} = \left(\begin{array}{ccccc|c} 1 & 0 & 0 & \dots & 0 & \\ 0 & 1 & 0 & \dots & 0 & \\ \dots & \dots & \dots & \dots & \dots & \boldsymbol{0} \\ 0 & 0 & 0 & \dots & 1 & \\ \hline & & \boldsymbol{0} & & & \boldsymbol{0} \end{array}\right) \begin{array}{l} \mathrm{m}-\mathrm{r} \\ \\ \\ \\ \mathrm{r} \end{array} \qquad (8.14)$$

$$\mathrm{m}-\mathrm{r} \qquad\qquad \mathrm{r}$$

Then, introducing an auxiliary vector

$$\boldsymbol{y} = (y_1 \quad y_2 \quad \dots \quad y_m)^{\mathrm{T}}$$

and putting

$$\frac{\boldsymbol{x}-\boldsymbol{\mu}}{\sigma} = \boldsymbol{T}\boldsymbol{y}\,,$$

(8.13) changes into

$$\bar{Q}_{\mathrm{weighted}} = (\boldsymbol{T}\boldsymbol{y})^{\mathrm{T}}\,(\boldsymbol{I}-\boldsymbol{P})\,\boldsymbol{T}\boldsymbol{y} = \sum_{i=1}^{m-r} y_i^2\,. \qquad (8.15)$$

The elements of the vector

$$\boldsymbol{y} = \boldsymbol{T}^{\mathrm{T}}\,(\boldsymbol{x}-\boldsymbol{\mu})\,/\sigma$$

are normally distributed. Moreover, on account of

$$E\,\{\boldsymbol{y}\} = \boldsymbol{0} \quad \text{and} \quad E\left\{\boldsymbol{y}\boldsymbol{y}^{\mathrm{T}}\right\} = \boldsymbol{T}^{\mathrm{T}}\boldsymbol{T} = \boldsymbol{I}\,,$$

they are standardized and independent. Thus, according to (8.15), $\bar{Q}_{\mathrm{weighted}}$ is χ^2-distributed with $m-r$ degrees of freedom, i.e.

$$E\left\{\bar{Q}_{\mathrm{weighted}}\right\} = m-r \quad \text{or} \quad E\,\{Q_{\mathrm{unweighted}}\} = \sigma^2\,(m-r)\;, \qquad (8.16)$$

see Sect. 3.3. Unfortunately, we are not allowed to ignore the term $(\boldsymbol{f}-\boldsymbol{P}\boldsymbol{f})$ in (8.12). As a consequence we find

$$E\,\{Q_{\mathrm{unweighted}}\} = \sigma^2\,(m-r) + \left(\boldsymbol{f}^{\mathrm{T}}\boldsymbol{f} - \boldsymbol{f}^{\mathrm{T}}\boldsymbol{P}\boldsymbol{f}\right) \qquad (8.17)$$

and this, obviously, means that as long as the second term on the right-hand side does not vanish, the experimenter is not in a position to derive an estimator for the variance of the input data from the minimized sum of squared residuals. In other words, provided that measurement uncertainties are considered indispensable, in general there is no chance of carrying out least squares adjustments based on single observations. In Sect. 10.1, however, we shall meet an exception.

Meanwhile, instead of using single observations $x_1, x_2, \ldots, x_m$, the experimenter may refer to arithmetic means

$$\bar{x}_1, \bar{x}_2, \ldots, \bar{x}_m\,; \quad \bar{x}_i = \frac{1}{n}\sum_{l=1}^{n} x_{il} \tag{8.18}$$

the empirical variances of which

$$s_i^2 = \frac{1}{n-1}\sum_{l=1}^{n}(x_{il} - \bar{x}_i)^2\,; \quad i = 1, \ldots, m \tag{8.19}$$

are known from the outset. Hence, we shall treat inconsistent systems of the kind

$$\boldsymbol{A}\boldsymbol{\beta} \approx \bar{\boldsymbol{x}}\,, \tag{8.20}$$

in which the components of the input vector $\bar{\boldsymbol{x}}$ are arithmetic means

$$\bar{x}_i = x_{0,i} + (\bar{x}_i - \mu_i) + f_i; \quad i = 1, \ldots, m\,. \tag{8.21}$$

In particular, we shall assume each mean to cover the same number n of repeat measurements. Just this ideas will enable us to assign a complete empirical variance–covariance matrix to the solution vector

$$\bar{\boldsymbol{\beta}} = \left(\boldsymbol{A}^{\mathrm{T}}\boldsymbol{A}\right)^{-1}\boldsymbol{A}^{\mathrm{T}}\bar{\boldsymbol{x}} = \boldsymbol{B}^{\mathrm{T}}\bar{\boldsymbol{x}}\,; \quad \boldsymbol{B} = \boldsymbol{A}\left(\boldsymbol{A}^{\mathrm{T}}\boldsymbol{A}\right)^{-1}\,. \tag{8.22}$$

8.3 Gauss–Markoff Theorem

As is well known, the concept of so-called "optimal estimators" frequently referred to in measurement technique is due to the Gauss–Markoff theorem.[1] Just for completeness let us present the theorem, temporarily ignoring the existence of systematic errors so that the least squares estimators are unbiased. The Gauss–Markoff theorem derives the uncertainties of the components of the least squares solution vector

$$\bar{\boldsymbol{\beta}} = (\bar{\beta}_1 \quad \bar{\beta}_2 \quad \cdots \quad \bar{\beta}_r)^{\mathrm{T}}$$

from the diagonal elements of the associated theoretical variance–covariance matrix

[1] R.L. Plackett (Biometrika, (1949), 149–157) has pointed out that the theorem is due to Gauss (*Theoria combinationis observationum erroribus minimis obnoxiae*, 1821/23). Presumably, the notation Gauss–Markoff theorem intends to honor Markoff's later contributions to the theory of least squares.

$$E\left\{\left(\bar{\boldsymbol{\beta}}-\boldsymbol{\mu}_{\bar{\beta}}\right)\left(\bar{\boldsymbol{\beta}}-\boldsymbol{\mu}_{\bar{\beta}}\right)^{\mathrm{T}}\right\}=\begin{pmatrix}\sigma_{\bar{\beta}_1\bar{\beta}_1} & \sigma_{\bar{\beta}_1\bar{\beta}_2} & \dots & \sigma_{\bar{\beta}_1\bar{\beta}_r}\\ \sigma_{\bar{\beta}_2\bar{\beta}_1} & \sigma_{\bar{\beta}_2\bar{\beta}_2} & \dots & \sigma_{\bar{\beta}_2\bar{\beta}_r}\\ \dots & \dots & \dots & \dots\\ \sigma_{\bar{\beta}_r\bar{\beta}_1} & \sigma_{\bar{\beta}_r\bar{\beta}_2} & \dots & \sigma_{\bar{\beta}_r\bar{\beta}_r}\end{pmatrix}. \tag{8.23}$$

If need be, we shall set $\sigma_{\bar{\beta}_k\bar{\beta}_k}\equiv\sigma^2_{\bar{\beta}_k}$. The uncertainties $u_{\bar{\beta}_k}$ of the components $\bar{\beta}_k$; $k=1,\dots,r$ would be

$$u_{\bar{\beta}_k}=\sqrt{\sigma_{\bar{\beta}_k\bar{\beta}_k}}\equiv\sigma_{\bar{\beta}_k}\,;\quad k=1,\dots,r\,.$$

The Gauss–Markoff theorem states:

Among all unbiased estimators, being linear in the input data, the least squares estimator minimizes the diagonal elements of the theoretical variance–covariance matrix of the solution vector.

In view of the underlying error model, however, least squares estimators are biased. In this respect, the fate of the theorem should be sealed. On the other hand, as the *ISO Guide* steadfastly continues to take the validity of the theorem for granted, we shall carry out computer simulations in order to settle the issue. As we shall see, the results not only differ in the sizes of the measurement uncertainties – an observation apparently regarded as disputable on the part of experimenters – but still in another property which, in fact, manoeuvres the *Guide* in a difficult position, see Sects. 8.4 and 9.3.

Ignoring systematic errors and assuming observations of equal accuracy, we have

$$E\left\{\left(\bar{\boldsymbol{x}}-\boldsymbol{x}_0\right)\left(\bar{\boldsymbol{x}}-\boldsymbol{x}_0\right)^{\mathrm{T}}\right\}=\frac{\sigma^2}{n}\,\boldsymbol{I}\,, \tag{8.24}$$

with $\boldsymbol{I}$ denoting an $(m\times m)$ identity matrix. According to (8.8) we have $\boldsymbol{\mu}_{\bar{\beta}}=\boldsymbol{\beta}_0$. But then (8.23) yields

$$E\left\{\left(\bar{\boldsymbol{\beta}}-\boldsymbol{\beta}_0\right)\left(\bar{\boldsymbol{\beta}}-\boldsymbol{\beta}_0\right)^{\mathrm{T}}\right\}=\frac{\sigma^2}{n}\left(\boldsymbol{A}^{\mathrm{T}}\boldsymbol{A}\right)^{-1}. \tag{8.25}$$

Instead of $\boldsymbol{B}=\boldsymbol{A}(\boldsymbol{A}^{\mathrm{T}}\boldsymbol{A})^{-1}$ let us impute the existence of an $(r\times m)$ matrix $\boldsymbol{V}$ defining another solution vector

$$\boldsymbol{\gamma}=\boldsymbol{V}\bar{\boldsymbol{x}} \tag{8.26}$$

of $\boldsymbol{A}\boldsymbol{\beta}\approx\bar{\boldsymbol{x}}$, also being linear in the observations. Of course, we ask for

$$\boldsymbol{\gamma}_0=\boldsymbol{V}\boldsymbol{x}_0=\boldsymbol{V}\boldsymbol{A}\boldsymbol{\beta}_0=\boldsymbol{\beta}_0\,;\quad\text{i.e.}\quad\boldsymbol{V}\boldsymbol{A}=\boldsymbol{I}\,. \tag{8.27}$$

As

$$E\left\{\left(\boldsymbol{\gamma}-\boldsymbol{\gamma}_0\right)\left(\boldsymbol{\gamma}-\boldsymbol{\gamma}_0\right)^{\mathrm{T}}\right\}=\frac{\sigma^2}{n}\boldsymbol{V}\boldsymbol{V}^{\mathrm{T}}\,,$$

we have to compare the diagonal elements of the variance–covariance matrices $(\boldsymbol{A}^{\mathrm{T}}\boldsymbol{A})^{-1}$ and $\boldsymbol{V}\boldsymbol{V}^{\mathrm{T}}$. The identity

$$\boldsymbol{V}\boldsymbol{V}^{\mathrm{T}} = \left(\boldsymbol{A}^{\mathrm{T}}\boldsymbol{A}\right)^{-1} + \left(\boldsymbol{V} - \boldsymbol{B}^{\mathrm{T}}\right)\left(\boldsymbol{V} - \boldsymbol{B}^{\mathrm{T}}\right)^{\mathrm{T}} \tag{8.28}$$

reveals the diagonal elements of $\boldsymbol{V}\boldsymbol{V}^{\mathrm{T}}$ to be non-negative; in particular they turn out to be minimal in case $\boldsymbol{V} = \boldsymbol{B}^{\mathrm{T}}$, i.e. if $\boldsymbol{V}$ is due to least squares.

However, we are not allowed to ignore the third term $\boldsymbol{B}^{\mathrm{T}}\boldsymbol{f}$ in (8.6). Consequently, the estimator $\bar{\boldsymbol{\beta}}$ is no longer unbiased and just this fact violates the Gauss–Markoff theorem. With respect to the error model under discussion we state:

Empirical data, being biased by unknown systematic errors, cause the Gauss–Markoff theorem to break down.

Nevertheless, let us continue to consider the classical form of an adjustment for a weighted linear system

$$\boldsymbol{G}\boldsymbol{A}\boldsymbol{\beta} \approx \boldsymbol{G}\bar{\boldsymbol{x}}\,. \tag{8.29}$$

According to the Gauss–Markoff theorem the optimal matrix of weights would be

$$\boldsymbol{G} = \left[E\left\{\left(\bar{\boldsymbol{x}} - \boldsymbol{x}_0\right)\left(\bar{\boldsymbol{x}} - \boldsymbol{x}_0\right)^{\mathrm{T}}\right\}\right]^{-1/2} \tag{8.30}$$

leading to minimal diagonal elements of the theoretical variance–covariance matrix

$$E\left\{\left(\bar{\boldsymbol{\beta}} - \boldsymbol{\beta}_{\mathbf{0}}\right)\left(\bar{\boldsymbol{\beta}} - \boldsymbol{\beta}_{\mathbf{0}}\right)^{\mathrm{T}}\right\} = \left[\left(\boldsymbol{G}\boldsymbol{A}\right)^{\mathrm{T}}\left(\boldsymbol{G}\boldsymbol{A}\right)\right]^{-1} \tag{8.31}$$

of the solution vector

$$\bar{\boldsymbol{\beta}} = \tilde{\boldsymbol{B}}^{\mathrm{T}}\boldsymbol{G}\bar{\boldsymbol{x}}\,, \quad \tilde{\boldsymbol{B}} = \left(\boldsymbol{G}\boldsymbol{A}\right)\left[\left(\boldsymbol{G}\boldsymbol{A}\right)^{\mathrm{T}}\left(\boldsymbol{G}\boldsymbol{A}\right)\right]^{-1} \tag{8.32}$$

of the weighted system (8.29). However, as Sect. 9.3 will disclose, these considerations turn out to be inoperative so that we shall have to proceed differently.

Incidentally, for the purposes of the experimenter, the Gauss–Markoff theorem does not seem to be exhaustive insofar as it presumes an invariable design matrix. On the other hand, it might well happen that one and the same measuring problem allows for quite different design matrices leading to varying measurement uncertainties. Unfortunately, the Gauss–Markoff theorem will in no way assist the experimenter in finding a design matrix generating absolutely minimal diagonal elements [20].

8.4 Choice of Weights

In general, the input data of the linear system

$$\boldsymbol{A}\boldsymbol{\beta} \approx \bar{\boldsymbol{x}} \tag{8.33}$$

will not be of the same accuracy. To boost the influence of more accurate data and reduce the influence of less accurate data, so-called weights should be introduced. Weighting the linear system means to multiply its m rows

$$\alpha_{i1}\beta_1 + \alpha_{i2}\beta_2 + \cdots + \alpha_{ir}\beta_r \approx \bar{x}_i\,; \quad i = 1, \ldots, m \tag{8.34}$$

by some factors $g_i \neq 0$.[2] We purposefully assemble the latter within a (non-singular) diagonal weight matrix

$$\boldsymbol{G} = \mathrm{diag}\,\{g_1, g_2, \ldots, g_m\}\ . \tag{8.35}$$

We emphasize that weights, in principle, do not shift the components of the true solution vector $\boldsymbol{\beta}_0$. Clearly,

$$\boldsymbol{G}\boldsymbol{A}\boldsymbol{\beta}_0 = \boldsymbol{G}\boldsymbol{x}_0 \tag{8.36}$$

re-establishes

$$\boldsymbol{\beta}_0 = \left[(\boldsymbol{G}\boldsymbol{A})^{\mathrm{T}}\,(\boldsymbol{G}\boldsymbol{A})\right]^{-1}(\boldsymbol{G}\boldsymbol{A})^{\mathrm{T}}\,\boldsymbol{G}\boldsymbol{x}_0 \tag{8.37}$$

regardless of the weights the experimenter has chosen. Mathematically, this property is self-evident. Nevertheless, it will turn out to be of crucial importance when measurement uncertainties are to be optimized, i.e. minimized.

Weighting procedures, however, shift the least squares estimators of the inconsistent linear system. Then, finding "points of attack", weights have two types of consequences: they

- shift the components of the vector $\bar{\boldsymbol{\beta}}$ and they
- either expand or compress the respective uncertainties.

Assuming the unknown systematic errors to abrogate the Gauss–Markoff theorem, there no longer is a rule of how to select the weight factors in order to minimize measurement uncertainties. Nevertheless, as will be demonstrated, the alternative error model is in a position to state:

The intervals

$$\bar{\beta}_k \pm u_{\bar{\beta}_k}\,; \quad k = 1, \ldots, r \tag{8.38}$$

localize the true values $\beta_{0,k}$ of the components $\bar{\beta}_k$ of the solution vector $\bar{\boldsymbol{\beta}}$ for any choice of the weights.

In a sense, this statement restores the memory of the method of least squares, see also Sect. 9.3. According to this result, we are, in principle, free to choose the weights g_i. In the standard case we would derive the weights from the uncertainties of the input data $\bar{x}_i$ through

[2] Even linear combinations of rows are admissible.

$$g_i = \frac{1}{u_{\bar{x}_i}}\,; \quad u_{\bar{x}_i} = \frac{t_P\,(n-1)}{\sqrt{n}} s_i + f_{s,i}\,; \quad i = 1, \ldots, m\,. \tag{8.39}$$

Beyond, we may cyclically repeat the numerical calculations varying the weights by trial and error and observe the estimator's uncertainties. Hence, we can see whether re-evaluation has produced larger or smaller uncertainties.

If the individual weights were multiplied by one and the same arbitrary factor, nothing would change. For instance, the g_i might be replaced with

$$\sqrt{w_i} = \frac{g_i}{\sqrt{\sum\limits_{i=1}^{m} g_i^2}}\,. \tag{8.40}$$

Clearly, the so-defined weights are dimensionless and their squares add up to one. But it remains immaterial to which set of weights we refer.

8.5 Consistency of the Input Data

Conventional least squares provides a test that shall reveal whether or not the input data are consistent,[3] i.e. whether they might be blurred by undetected systematic errors.[4] In the presence of unknown systematic errors, any such test will, of course, be superfluous. Nevertheless, we shall derive it, though, basically, it simply is a repetition of the considerations of Sect. 8.2. Let the input data be arithmetic means

$$\bar{\boldsymbol{x}} = (\bar{x}_1 \quad \bar{x}_2 \quad \cdots \quad \bar{x}_m)^{\mathrm{T}}\,. \tag{8.41}$$

Their underlying theoretical variances

$$\sigma_i^2 = E\left\{(X_i - \mu_i)^2\right\}\,; \quad i = 1, \ldots, m \tag{8.42}$$

may be different. Conventional least squares obtains the weight matrix $\boldsymbol{G}$ from the Gauss–Markoff theorem, i.e. from the theoretical variance–covariance matrix of the input data,

$$E\left\{(\bar{\boldsymbol{x}} - \boldsymbol{\mu})\,(\bar{\boldsymbol{x}} - \boldsymbol{\mu})^{\mathrm{T}}\right\} = \frac{1}{n}\begin{pmatrix} \sigma_{11} & \sigma_{12} & \ldots & \sigma_{1m} \\ \sigma_{21} & \sigma_{22} & \ldots & \sigma_{2m} \\ \ldots & \ldots & \ldots & \ldots \\ \sigma_{m1} & \sigma_{m2} & \ldots & \sigma_{mm} \end{pmatrix}\,; \quad \sigma_{ii} \equiv \sigma_i^2\,, \tag{8.43}$$

[3] From our point of view, consistency means that the relationship between the true values of the input data and the true solution vector is physically unique.

[4] Undetected simply means that it has not been known to the experimenter that an unknown systematic error he should have taken into account has been operative.

setting

$$\boldsymbol{G} = \left[E\left\{ (\bar{\boldsymbol{x}} - \boldsymbol{\mu}) (\bar{\boldsymbol{x}} - \boldsymbol{\mu})^{\mathrm{T}} \right\} \right]^{-1/2} . \tag{8.44}$$

Multiplying the inconsistent linear system

$$\boldsymbol{A\beta} \approx \bar{\boldsymbol{x}} \tag{8.45}$$

on the left by $\boldsymbol{G}$ yields

$$\boldsymbol{GA\beta} \approx \boldsymbol{G}\bar{\boldsymbol{x}} . \tag{8.46}$$

The projection operator and the vector of the residuals are given by

$$\boldsymbol{P} = (\boldsymbol{GA}) \left[(\boldsymbol{GA})^{\mathrm{T}} (\boldsymbol{GA}) \right]^{-1} (\boldsymbol{GA})^{\mathrm{T}} \tag{8.47}$$

and

$$\bar{\boldsymbol{r}} = \boldsymbol{G}\bar{\boldsymbol{x}} - \boldsymbol{PG}\bar{\boldsymbol{x}} \tag{8.48}$$

respectively. Inserting

$$\bar{\boldsymbol{x}} = \boldsymbol{x}_0 + (\bar{\boldsymbol{x}} - \boldsymbol{\mu}) + \boldsymbol{f} \tag{8.49}$$

we find

$$\bar{\boldsymbol{r}} = \boldsymbol{G} (\bar{\boldsymbol{x}} - \boldsymbol{\mu}) - \boldsymbol{PG} (\bar{\boldsymbol{x}} - \boldsymbol{\mu}) + (\boldsymbol{Gf} - \boldsymbol{PGf}) , \tag{8.50}$$

since[5]

$$\boldsymbol{PGx_0} = \boldsymbol{Gx_0} . \tag{8.51}$$

Disregarding systematic errors in (8.50), i.e. the third term on the right, the minimized sum of squared residuals is given by

$$\bar{Q}_{\mathrm{weighted}} = \bar{\boldsymbol{r}}^{\mathrm{T}} \bar{\boldsymbol{r}} = \left[\boldsymbol{G} (\bar{\boldsymbol{x}} - \boldsymbol{\mu}) \right]^{\mathrm{T}} (\boldsymbol{I} - \boldsymbol{P}) \left[\boldsymbol{G} (\bar{\boldsymbol{x}} - \boldsymbol{\mu}) \right] , \tag{8.52}$$

where $\boldsymbol{I}$ designates an $(m \times m)$ identity matrix. Let $\boldsymbol{T}$ denote an orthogonal $(m \times m)$ matrix and $\bar{\boldsymbol{y}}$ an $(m \times 1)$ auxiliary vector. Putting

$$\boldsymbol{G} (\bar{\boldsymbol{x}} - \boldsymbol{\mu}) = \boldsymbol{T}\bar{\boldsymbol{y}}; \quad \bar{\boldsymbol{y}} = \boldsymbol{T}^{\mathrm{T}} \boldsymbol{G} (\bar{\boldsymbol{x}} - \boldsymbol{\mu}) \tag{8.53}$$

and referring to (8.14) we find

$$\bar{Q}_{\mathrm{weighted}} = (\boldsymbol{T}\bar{\boldsymbol{y}})^{\mathrm{T}} (\boldsymbol{I} - \boldsymbol{P}) \boldsymbol{T}\bar{\boldsymbol{y}} = \sum_{i=1}^{m-r} \bar{y}_i^2 . \tag{8.54}$$

[5] Following (8.36) the vector $\boldsymbol{Gx_0}$ is an element of the column space of the matrix $\boldsymbol{GA}$. According to (8.47), the operator $\boldsymbol{P}$ projects onto this space.

Again, the components of the auxiliary vector $\bar{\boldsymbol{y}}$ are normally distributed (even if there are dependencies between the means $\bar{x}_i$, see Appendix C, [40]). As

$$E\{\bar{\boldsymbol{y}}\} = \boldsymbol{0} \quad \text{and} \quad E\left\{\bar{\boldsymbol{y}}\bar{\boldsymbol{y}}^{\mathrm{T}}\right\} = \boldsymbol{T}^{\mathrm{T}}\boldsymbol{T} = \boldsymbol{I}\,,$$

$\bar{Q}_{\text{weighted}}$ is χ^2-distributed with $m - r$ degrees of freedom, i.e.

$$E\left\{\bar{Q}_{\text{weighted}}\right\} = m - r\,.$$

After all, given that the input data are free from systematic errors we should observe

$$\bar{Q}_{\text{weighted}} \approx m - r\,. \tag{8.55}$$

Meanwhile, accounting for the term $(\boldsymbol{G}\boldsymbol{f} - \boldsymbol{P}\boldsymbol{G}\boldsymbol{f})$ disregarded in (8.50), and the observation that, due to systematic errors, the weight matrix $\boldsymbol{G}$ as proposed in (8.35) should be used, we have instead

$$E\left\{\bar{Q}_{\text{weighted}}\right\} = \sum_{i=1}^{m} g_i^2 \frac{\sigma_i^2}{n} - \sum_{i=1}^{m} g_i^2 \frac{\sigma_i^2}{n} p_{ii} + \left[(\boldsymbol{G}\boldsymbol{f})^{\mathrm{T}}(\boldsymbol{G}\boldsymbol{f}) - (\boldsymbol{G}\boldsymbol{f})^{\mathrm{T}}\boldsymbol{P}(\boldsymbol{G}\boldsymbol{f})\right]. \tag{8.56}$$

Here, the p_{ii} designate the diagonal elements of the projection matrix $\boldsymbol{P}$ introduced in (8.47). We note that (8.56) presupposes independent $\bar{x}_i$ as otherwise the expected value $E\{\bar{Q}_{\text{weighted}}\}$ would turn out to be more complex. We observe:

Unknown systematic errors suspend the property of the weighted minimized sum of squared residuals to estimate the number of the degrees of freedom of the linear system.

For decades empirical observations, in particular those relating to high-level metrology, have revealed over and over again

$$\bar{Q}_{\text{weighted}} \gg m - r\,, \tag{8.57}$$

[16,17]. Procedures relying on the *ISO Guide* [36] then speak of inconsistent input data attributing the inconsistencies to *undetected* unknown systematic errors. However, within the alternative error model, (8.57) does not necessarily express inconsistencies among the input data, as we think (8.56) rather than (8.55) applies. Whether or not measuring data are inconsistent should be scrutinized by other means.

9 Uncertainties of Least Squares Estimators

9.1 Empirical Variance–Covariance Matrix

To determine the uncertainties of the least squares estimators, we resort to the decomposition (8.6),

$$\bar{\boldsymbol{\beta}} = \boldsymbol{B}^{\mathrm{T}}\bar{\boldsymbol{x}} = \boldsymbol{B}^{\mathrm{T}}\left[\boldsymbol{x}_0 + (\bar{\boldsymbol{x}} - \boldsymbol{\mu}) + \boldsymbol{f}\right] . \tag{9.1}$$

Let us firstly estimate the term $\boldsymbol{B}^{\mathrm{T}}(\bar{\boldsymbol{x}} - \boldsymbol{\mu})$. In contrast to the conventional error calculus, we shall rely on empirical quantities, i.e. we shall establish the empirical variance–covariance matrix direct from the input data. This is possible, given each of the $\bar{x}_i$; $i = 1, \ldots, m$ relates to the same number of repeat measurements, as was presumed. Then, the said matrix allows us to express those parts of the overall uncertainties which are due to random errors through confidence intervals according to Student. In principle, we shall proceed as in Sect. 6.3 starting from the components $\bar{\beta}_k$; $k = 1, \ldots, r$ of the estimator (9.1). Denoting the elements of the matrix $\boldsymbol{B}$ by b_{ik},

$$\boldsymbol{B} = \boldsymbol{A}(\boldsymbol{A}^{\mathrm{T}}\boldsymbol{A})^{-1} = (b_{ik}) \ , \quad i = 1, \ldots, m \, ; \, k = 1, \ldots, r \, ,$$

we find from

$$\bar{\beta}_k = \sum_{i=1}^{m} b_{ik}\bar{x}_i \, ; \quad k = 1, \ldots, r \, , \tag{9.2}$$

inserting the means

$$\bar{x}_i = \frac{1}{n}\sum_{l=1}^{n} x_{il} \, ,$$

the representations

$$\bar{\beta}_k = \sum_{i=1}^{m} b_{ik}\left[\frac{1}{n}\sum_{l=1}^{n} x_{il}\right] = \frac{1}{n}\sum_{l=1}^{n}\left[\sum_{i=1}^{m} b_{ik}x_{il}\right]$$

$$= \frac{1}{n}\sum_{l=1}^{n} \bar{\beta}_{kl} \, ; \quad k = 1, \ldots, r \, . \tag{9.3}$$

For convenience, the sums

$$\bar{\beta}_{kl} = \sum_{i=1}^{m} b_{ik} x_{il}\,; \quad k = 1, \ldots, r \tag{9.4}$$

may be understood as components of a least squares estimator, the input data of which are the m individual measurements $x_{1l}, x_{2l}, \ldots, x_{ml}$: each of the m means $\bar{x}_i$ contributes just the l-th measured datum. The following illustration depicts the situation:

$$\begin{array}{ccccccccc}
x_{11} & x_{12} & \ldots & x_{1l} & \ldots & x_{1n} & \Rightarrow & \bar{x}_1 \\
x_{21} & x_{22} & \ldots & x_{2l} & \ldots & x_{2n} & \Rightarrow & \bar{x}_2 \\
\ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots \\
x_{m1} & x_{m2} & \ldots & x_{ml} & \ldots & x_{mn} & \Rightarrow & \bar{x}_m \\
\Downarrow & \Downarrow & & \Downarrow & & \Downarrow & & \Downarrow \\
\bar{\beta}_{k1} & \bar{\beta}_{k2} & & \bar{\beta}_{kl} & & \bar{\beta}_{kn} & \Rightarrow & \bar{\beta}_k
\end{array}$$

According to (9.3), the $\bar{\beta}_k$ are the arithmetic means of the n means $\bar{\beta}_{kl}$. The differences

$$\bar{\beta}_{kl} - \bar{\beta}_k = \sum_{i=1}^{m} b_{ik} \left(x_{il} - \bar{x}_i\right)\,; \quad l = 1, \ldots, n;\; k = 1, \ldots, r \tag{9.5}$$

allow us to establish the empirical variances and covariances

$$s_{\bar{\beta}_k \bar{\beta}_{k'}} = \frac{1}{n-1} \sum_{l=1}^{n} \left(\bar{\beta}_{kl} - \bar{\beta}_k\right) \left(\bar{\beta}_{k'l} - \bar{\beta}_{k'}\right); \quad k, k' = 1, \ldots, r$$

of the components of the estimator $\bar{\boldsymbol{\beta}}$ and thus its empirical variance–covariance matrix

$$\boldsymbol{s}_{\bar{\boldsymbol{\beta}}} = \begin{pmatrix}
s_{\bar{\beta}_1 \bar{\beta}_1} & s_{\bar{\beta}_1 \bar{\beta}_2} & \ldots & s_{\bar{\beta}_1 \bar{\beta}_r} \\
s_{\bar{\beta}_2 \bar{\beta}_1} & s_{\bar{\beta}_2 \bar{\beta}_2} & \ldots & s_{\bar{\beta}_2 \bar{\beta}_r} \\
\ldots & \ldots & \ldots & \ldots \\
s_{\bar{\beta}_r \bar{\beta}_1} & s_{\bar{\beta}_r \bar{\beta}_2} & \ldots & s_{\bar{\beta}_r \bar{\beta}_r}
\end{pmatrix}\,; \quad s_{\bar{\beta}_k \bar{\beta}_k} \equiv s^2_{\bar{\beta}_k}\,. \tag{9.6}$$

Inserting the differences (9.5) into $s_{\bar{\beta}_k \bar{\beta}_{k'}}$, we obtain

$$\begin{aligned}
s_{\bar{\beta}_k \bar{\beta}_{k'}} &= \frac{1}{n-1} \sum_{l=1}^{n} \left[\sum_{i=1}^{m} b_{ik} \left(x_{il} - \bar{x}_i\right)\right] \left[\sum_{j=1}^{m} b_{jk'} \left(x_{jl} - \bar{x}_j\right)\right] \\
&= \sum_{i,j}^{m} b_{ik} b_{jk'} s_{ij}\,.
\end{aligned} \tag{9.7}$$

Here the quantities

$$s_{ij} = \frac{1}{n-1} \sum_{l=1}^{n} (x_{il} - \bar{x}_i)\,(x_{jl} - \bar{x}_j)\ ; \quad i, j = 1, \ldots, m \tag{9.8}$$

designate the elements of the empirical variance–covariance matrix of the input data

$$\boldsymbol{s} = \begin{pmatrix} s_{11} & s_{12} & \ldots & s_{1m} \\ s_{21} & s_{22} & \ldots & s_{2m} \\ \ldots & \ldots & \ldots & \ldots \\ s_{m1} & s_{m2} & \ldots & s_{mm} \end{pmatrix} . \tag{9.9}$$

By means of the column vectors $\boldsymbol{b}_k$; $k = 1, \ldots, r$ of the matrix $\boldsymbol{B}$,

$$\boldsymbol{B} = (\boldsymbol{b}_1\, \boldsymbol{b}_2 \cdots \boldsymbol{b}_r)\ , \tag{9.10}$$

we can compress the variances and covariances as defined in (9.7) into

$$\boldsymbol{s}_{\bar{\boldsymbol{\beta}}_k \bar{\boldsymbol{\beta}}_{k'}} = \boldsymbol{b}_k^{\mathrm{T}} \boldsymbol{s}\, \boldsymbol{b}_{k'}\ ; \quad k,\, k' = 1, \ldots, r\,. \tag{9.11}$$

Hence, (9.6) turns into

$$\boldsymbol{s}_{\bar{\beta}} = \begin{pmatrix} \boldsymbol{b}_1^{\mathrm{T}} \boldsymbol{s}\, \boldsymbol{b}_1 & \boldsymbol{b}_1^{\mathrm{T}} \boldsymbol{s}\, \boldsymbol{b}_2 & \ldots & \boldsymbol{b}_1^{\mathrm{T}} \boldsymbol{s}\, \boldsymbol{b}_r \\ \boldsymbol{b}_2^{\mathrm{T}} \boldsymbol{s}\, \boldsymbol{b}_1 & \boldsymbol{b}_2^{\mathrm{T}} \boldsymbol{s}\, \boldsymbol{b}_2 & \ldots & \boldsymbol{b}_2^{\mathrm{T}} \boldsymbol{s}\, \boldsymbol{b}_r \\ \ldots & \ldots & \ldots & \ldots \\ \boldsymbol{b}_r^{\mathrm{T}} \boldsymbol{s}\, \boldsymbol{b}_1 & \boldsymbol{b}_r^{\mathrm{T}} \boldsymbol{s}\, \boldsymbol{b}_2 & \ldots & \boldsymbol{b}_r^{\mathrm{T}} \boldsymbol{s}\, \boldsymbol{b}_r \end{pmatrix} = \boldsymbol{B}^{\mathrm{T}} \boldsymbol{s}\, \boldsymbol{B}\,. \tag{9.12}$$

As each of the $\bar{\beta}_k$; $k = 1, 2, \ldots, r$ relies on the same set of input data, they necessarily are dependent. The same applies to the $\bar{\beta}_{kl}$. Moreover, for any fixed i, the sequence of the x_{il} is indeterminate, i.e. we may interchange the x_{il}; i fixed. With these permutations, the $\bar{\beta}_k$ do not alter; the $\bar{\beta}_{kl}$, however, will alter. Consequently, the elements of the matrices (9.9) and (9.12) depend on the sequences of the x_{il}; i fixed. This, nevertheless, complies perfectly with the properties of the underlying statistical distributions and, in particular, with our aim of introducing Student's confidence intervals.

In order to find the empirical variance–covariance matrix of the weighted adjustment, we resort to (8.29)

$$\boldsymbol{G}\boldsymbol{A}\boldsymbol{\beta} \approx \boldsymbol{G}\bar{\boldsymbol{x}} = \boldsymbol{G}\,[\boldsymbol{x}_0 + (\bar{\boldsymbol{x}} - \boldsymbol{\mu}) + \boldsymbol{f}]$$

and (8.32)[1]

[1]Though the weighted solution vector $\bar{\boldsymbol{\beta}}$ will be different from the unweighted one, for simplicity, we use the same symbol.

$$\bar{\boldsymbol{\beta}} = \tilde{\boldsymbol{B}}^{\mathrm{T}} \boldsymbol{G} \bar{\boldsymbol{x}}\,; \quad \tilde{\boldsymbol{B}} = (\boldsymbol{G}\boldsymbol{A}) \left[(\boldsymbol{G}\boldsymbol{A})^{\mathrm{T}} (\boldsymbol{G}\boldsymbol{A}) \right]^{-1} .$$

Denoting the elements $\tilde{b}_{ik}$ of the $(m \times r)$ matrix $\tilde{\boldsymbol{B}}$ by $\tilde{b}_{ik}$, we write the r components $\bar{\beta}_k$ of the vector $\bar{\boldsymbol{\beta}}$ in the form

$$\bar{\beta}_k = \sum_{i=1}^{m} \tilde{b}_{ik} g_i \bar{x}_i\,; \quad k = 1, \ldots, r\,. \tag{9.13}$$

Insertion of

$$\bar{x}_i = \frac{1}{n} \sum_{l=1}^{n} x_{il}$$

leads to

$$\bar{\beta}_k = \sum_{i=1}^{m} \tilde{b}_{ik} g_i \left[\frac{1}{n} \sum_{l=1}^{n} x_{il} \right] = \frac{1}{n} \sum_{l=1}^{n} \left[\sum_{i=1}^{m} \tilde{b}_{ik} g_i x_{il} \right] = \frac{1}{n} \sum_{l=1}^{n} \bar{\beta}_{kl}\,. \tag{9.14}$$

Again, we may consider the quantities

$$\bar{\beta}_{kl} = \sum_{i=1}^{m} \tilde{b}_{ik} g_i x_{il} \tag{9.15}$$

as the components of a least squares estimator, the input data of which are the m weighted individual measurements $x_{1l}, x_{2l}, \ldots, x_{ml}$. Referring to the differences

$$\bar{\beta}_{kl} - \bar{\beta}_k = \sum_{i=1}^{m} \tilde{b}_{ik} g_i \left(x_{il} - \bar{x}_i \right)\,; \quad k = 1, \ldots, r\,,$$

we form the elements

$$\begin{aligned} s_{\bar{\beta}_k \bar{\beta}_{k'}} &= \frac{1}{n-1} \sum_{l=1}^{n} \left[\sum_{i=1}^{m} \tilde{b}_{ik} g_i \left(x_{il} - \bar{x}_i \right) \right] \left[\sum_{j=1}^{m} \tilde{b}_{jk'} g_j \left(x_{jl} - \bar{x}_j \right) \right] \\ &= \sum_{i,j}^{m} \tilde{b}_{ik} \tilde{b}_{jk'} g_i g_j s_{ij} \end{aligned} \tag{9.16}$$

of the empirical variance–covariance matrix $\boldsymbol{s}_{\bar{\beta}}$. The matrix itself is given by

$$\begin{aligned} \boldsymbol{s}_{\bar{\boldsymbol{\beta}}} &= \begin{pmatrix} \tilde{\boldsymbol{b}}_1^{\mathrm{T}} \left(\boldsymbol{G}^{\mathrm{T}} \boldsymbol{s}\, \boldsymbol{G} \right) \tilde{\boldsymbol{b}}_1 & \tilde{\boldsymbol{b}}_1^{\mathrm{T}} \left(\boldsymbol{G}^{\mathrm{T}} \boldsymbol{s}\, \boldsymbol{G} \right) \tilde{\boldsymbol{b}}_2 & \ldots & \tilde{\boldsymbol{b}}_1^{\mathrm{T}} \left(\boldsymbol{G}^{\mathrm{T}} \boldsymbol{s}\, \boldsymbol{G} \right) \tilde{\boldsymbol{b}}_r \\ \tilde{\boldsymbol{b}}_2^{\mathrm{T}} \left(\boldsymbol{G}^{\mathrm{T}} \boldsymbol{s}\, \boldsymbol{G} \right) \tilde{\boldsymbol{b}}_1 & \tilde{\boldsymbol{b}}_2^{\mathrm{T}} \left(\boldsymbol{G}^{\mathrm{T}} \boldsymbol{s}\, \boldsymbol{G} \right) \tilde{\boldsymbol{b}}_2 & \ldots & \tilde{\boldsymbol{b}}_2^{\mathrm{T}} \left(\boldsymbol{G}^{\mathrm{T}} \boldsymbol{s}\, \boldsymbol{G} \right) \tilde{\boldsymbol{b}}_r \\ \ldots & \ldots & \ldots & \ldots \\ \tilde{\boldsymbol{b}}_r^{\mathrm{T}} \left(\boldsymbol{G}^{\mathrm{T}} \boldsymbol{s}\, \boldsymbol{G} \right) \tilde{\boldsymbol{b}}_1 & \tilde{\boldsymbol{b}}_r^{\mathrm{T}} \left(\boldsymbol{G}^{\mathrm{T}} \boldsymbol{s}\, \boldsymbol{G} \right) \tilde{\boldsymbol{b}}_2 & \ldots & \tilde{\boldsymbol{b}}_r^{\mathrm{T}} \left(\boldsymbol{G}^{\mathrm{T}} \boldsymbol{s}\, \boldsymbol{G} \right) \tilde{\boldsymbol{b}}_r \end{pmatrix} \\ &= \tilde{\boldsymbol{B}}^{\mathrm{T}} \left(\boldsymbol{G}^{\mathrm{T}} \boldsymbol{s}\, \boldsymbol{G} \right) \tilde{\boldsymbol{B}}\,. \end{aligned} \tag{9.17}$$

Here, we have made use of

$$\tilde{\boldsymbol{B}} = \left(\tilde{\boldsymbol{b}}_1\, \tilde{\boldsymbol{b}}_2\, \cdots\, \tilde{\boldsymbol{b}}_r\right) = \left(\tilde{b}_{ik}\right)\,. \tag{9.18}$$

The elements s_{ij} and the matrix $\boldsymbol{s}$ have been defined in (9.8) and (9.9) respectively.

Each of the quantities $\bar{\beta}_{kl}$, as defined in (9.4) and (9.15), imply just one set of input data $x_{1l}, x_{2l}, \ldots, x_{ml}$. Assuming the successive sets $l = 1, 2, \ldots, n$ to be independent and assigning an m-dimensional normal density to each of them, we are in a position to introduce Student's confidence intervals. For the non-weighted adjustment we have

$$\bar{\beta}_k \pm \frac{t_P\,(n-1)}{\sqrt{n}} \sqrt{\sum_{i,j}^{m} b_{ik} b_{jk}\; s_{ij}}\,; \quad k = 1, \ldots, r \tag{9.19}$$

while the weighted adjustment yields

$$\bar{\beta}_k \pm \frac{t_P\,(n-1)}{\sqrt{n}} \sqrt{\sum_{i,j}^{m} \tilde{b}_{ik} \tilde{b}_{jk} g_i g_j\; s_{ij}}\,; \quad k = 1, \ldots, r\,. \tag{9.20}$$

The intervals (9.19) and (9.20) localize the components of the vectors

$$\boldsymbol{\mu}_{\bar{\boldsymbol{\beta}}} = \boldsymbol{\beta}_0 + \boldsymbol{B}^{\mathrm{T}} \boldsymbol{f} \tag{9.21}$$

and

$$\tilde{\boldsymbol{\mu}}_{\bar{\boldsymbol{\beta}}} = \boldsymbol{\beta}_0 + \tilde{\boldsymbol{B}}^{\mathrm{T}} \boldsymbol{G} \boldsymbol{f} \tag{9.22}$$

respectively, with probability P as given by $t_P\,(n-1)$.

9.2 Propagation of Systematic Errors

From (9.21) and (9.22) we read the systematic errors of the estimators of the non-weighted and the weighted adjustment respectively,

$$\boldsymbol{f}_{\bar{\boldsymbol{\beta}}} = \boldsymbol{B}^{\mathrm{T}} \boldsymbol{f}\,; \quad \tilde{\boldsymbol{f}}_{\bar{\boldsymbol{\beta}}} = \tilde{\boldsymbol{B}}^{\mathrm{T}} \boldsymbol{G} \boldsymbol{f}\,, \tag{9.23}$$

or, written in components,

$$f_{\bar{\beta}_k} = \sum_{i=1}^{m} b_{ik} f_i\,; \quad \tilde{f}_{\bar{\beta}_k} = \sum_{i=1}^{m} \tilde{b}_{ik} g_i f_i\,; \quad k = 1, \ldots, r\,. \tag{9.24}$$

Their worst-case estimations are

$$f_{s,\bar{\beta}_k} = \sum_{i=1}^{m} |b_{ik}|\, f_{s,i} \tag{9.25}$$

and

$$\tilde{f}_{s,\bar{\beta}_k} = \sum_{i=1}^{m} \left|\tilde{b}_{ik}\right| g_i f_{s,i}\,. \tag{9.26}$$

Should $f_i = f = \text{const.}$, $i = 1, \ldots, m$ apply, the estimations turn out to be more favorable,

$$f_{s,\bar{\beta}_k} = f_s \left|\sum_{i=1}^{m} b_{ik}\right| ; \quad \tilde{f}_{s,\bar{\beta}_k} = f_s \left|\sum_{i=1}^{m} \tilde{b}_{ik} g_i\right| . \tag{9.27}$$

According to (9.25) and (9.26), the new formalism should respond to an rising number m of input data with an inappropriate growth in the propagated systematic errors, thus blotting out the increase in input information. This would, of course, scarcely make sense. Fortunately, as the examples in Sect. 9.3 will underscore, this indeed does not apply. For now, let us make this observation a bit plausible. Suppressing the index k and confining ourselves to $m = 2$ so that

$$f_{\bar{\beta}} = b_1 f_1 + b_2 f_2\,,$$

we find from

$$f_{\bar{\beta}} = b_1 \bar{x}_1 \frac{f_1}{\bar{x}_1} + b_2 \bar{x}_2 \frac{f_2}{\bar{x}_2}\,,$$

dividing by $\bar{\beta} = b_1 \bar{x}_1 + b_2 \bar{x}_2$,

$$\frac{f_{\bar{\beta}}}{\bar{\beta}} = p_1 \frac{f_1}{\bar{x}_1} + p_2 \frac{f_2}{\bar{x}_2}\,,$$

where

$$p_1 = \frac{b_1 \bar{x}_1}{\bar{\beta}}\,; \quad p_2 = \frac{b_2 \bar{x}_2}{\bar{\beta}}\,; \quad p_1 + p_2 = 1\,.$$

As long as p_1 and p_2 act as true weight factors, being both positive, we have

$$\frac{f_{s,\bar{\beta}}}{|\bar{\beta}|} = p_1 \frac{f_{s,1}}{|\bar{x}_1|} + p_2 \frac{f_{s,2}}{|\bar{x}_2|}\,.$$

In general, however, the situation might not be that simple.

9.3 Overall Uncertainties of the Estimators

To find the overall uncertainties $u_{\bar{\beta}_k}$; $k = 1, \ldots, r$ of the least squares adjustment, we refer to the decomposition

$$\begin{aligned}\bar{\boldsymbol{\beta}} &= \tilde{\boldsymbol{B}}^{\mathrm{T}} \boldsymbol{G} \left[\boldsymbol{x}_0 + (\bar{\boldsymbol{x}} - \boldsymbol{\mu}) + \boldsymbol{f}\right] \\ &= \boldsymbol{\beta}_0 + \tilde{\boldsymbol{B}}^{\mathrm{T}} \boldsymbol{G} (\bar{\boldsymbol{x}} - \boldsymbol{\mu}) + \tilde{\boldsymbol{B}}^{\mathrm{T}} \boldsymbol{G} \boldsymbol{f} \,. \end{aligned} \tag{9.28}$$

As usual, we linearly combine the estimations (9.19), (9.25) and (9.20), (9.26) respectively, to obtain the quested uncertainty intervals

$$\bar{\beta}_k - u_{\bar{\beta}_k} \leq \beta_{0,\,k} \leq \bar{\beta}_k + u_{\bar{\beta}_k} \,; \quad k = 1, \ldots, r \,. \tag{9.29}$$

While the non-weighted adjustment yields

$$u_{\bar{\beta}_k} = \frac{t_P \,(n-1)}{\sqrt{n}} \sqrt{\sum_{i,j}^{m} b_{ik} b_{jk} s_{ij}} + \sum_{i=1}^{m} |b_{ik}| \, f_{s,i} \,, \tag{9.30}$$

the weighted adjustment issues

$$u_{\bar{\beta}_k} = \frac{t_P \,(n-1)}{\sqrt{n}} \sqrt{\sum_{i,j}^{m} \tilde{b}_{ik} \tilde{b}_{jk} g_i g_j s_{ij}} + \sum_{i=1}^{m} \left|\tilde{b}_{ik}\right| g_i f_{s,i} \,. \tag{9.31}$$

In either case, we expect the intervals (9.29) to localize the true values $\beta_{0,k}$ of the estimators $\bar{\beta}_k$; $k = 1, \ldots, r$. As Fig. 9.1 depicts, the least squares adjustment depends on

- the input data,
- the choice of the design matrix $\boldsymbol{A}$, and
- the structure of the weight matrix

Let us recall (see Sect. 8.4) that weightings involve two things: they numerically shift the estimators and they alter the pertaining uncertainties. Nonetheless, as the uncertainty intervals steadfastly localize the estimators' true values independent of which weights have been chosen, we may attribute something like a memory to the approach. Also, we should not cling so much to the numerical values of the estimators but rather consider intervals as quoted in (9.29). As Fig. 9.2 illustrates, we may assume a set of uncertainty intervals stemming from different experiments and aiming at one and the same physical quantity. Then, each of the intervals should localize the common true value $\beta_{0,k}$. In other words, the intervals should mutually overlap.

The property (9.29) proves to be of vital importance and differs significantly from the implications of the *ISO Guide*. Though the latter evens out inconsistencies among the input data, the experimenter must, unfortunately,

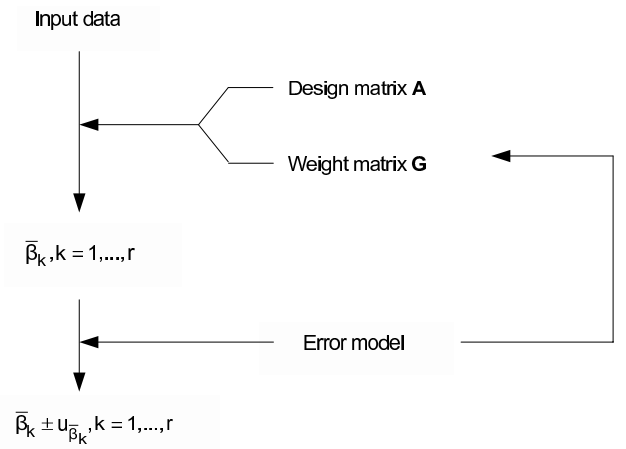


Fig. 9.1. The least squares adjustment depends on the input data, the design matrix $\boldsymbol{A}$ and the weight matrix $\boldsymbol{G}$. The latter may be chosen by trial and error to minimize the uncertainties of the estimators

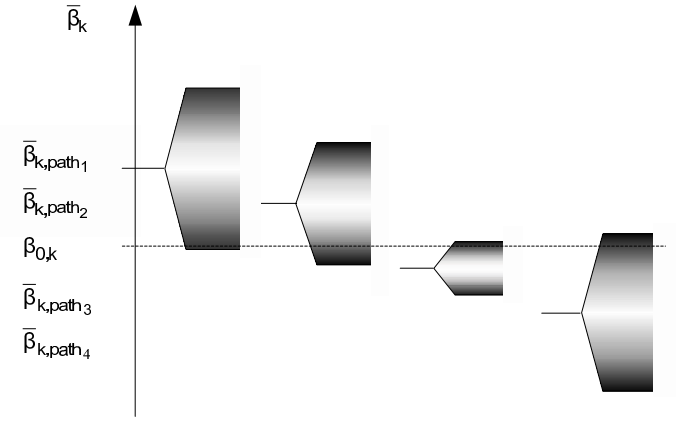


Fig. 9.2. Overlaps of uncertainty regions of measuring results coming from different paths and aiming at one and the same physical quantity $\beta_{0,k}$

be aware of the fact that the uncertainties at hand might not embrace the true values he is looking for.

Nonetheless, for completeness, we add the *Guide's* formalism: The linear system and the least squares estimator of the non-weighted adjustment are given by

$$\boldsymbol{A}\boldsymbol{\beta} \approx \bar{\boldsymbol{x}}\,, \quad \bar{\boldsymbol{\beta}} = \boldsymbol{B}^{\mathrm{T}}\bar{\boldsymbol{x}}\,, \quad \boldsymbol{B} = \boldsymbol{A}\left(\boldsymbol{A}^{\mathrm{T}}\boldsymbol{A}\right)^{-1} \tag{9.32}$$

where

$$\boldsymbol{\beta}_0 = E\left\{\bar{\boldsymbol{\beta}}\right\} = \boldsymbol{B}^{\mathrm{T}}\boldsymbol{x_0}$$

is tacitly assumed. But then, the theoretical variance–covariance matrix of the estimator $\bar{\boldsymbol{\beta}}$ would be

$$E\left\{\left(\bar{\boldsymbol{\beta}}-\boldsymbol{\beta}_0\right)\left(\bar{\boldsymbol{\beta}}-\boldsymbol{\beta}_0\right)^{\mathrm{T}}\right\}=\boldsymbol{B}^{\mathrm{T}}E\left\{\left(\bar{\boldsymbol{x}}-\boldsymbol{x}_0\right)\left(\bar{\boldsymbol{x}}-\boldsymbol{x}_0\right)^{\mathrm{T}}\right\}\boldsymbol{B}\,. \tag{9.33}$$

The square roots of its diagonal elements are seen to be the uncertainties of the non-weighted adjustment. Similarly, for the weighted adjustment we have

$$\boldsymbol{G}\boldsymbol{A}\,\boldsymbol{\beta}\approx\boldsymbol{G}\,\bar{\boldsymbol{x}}\,,\quad \bar{\boldsymbol{\beta}}=\tilde{\boldsymbol{B}}^{\mathrm{T}}\boldsymbol{G}\,\bar{\boldsymbol{x}}\,,\quad \tilde{\boldsymbol{B}}=\left(\boldsymbol{G}\boldsymbol{A}\right)\left[\left(\boldsymbol{G}\boldsymbol{A}\right)^{\mathrm{T}}\left(\boldsymbol{G}\boldsymbol{A}\right)\right]^{-1} \tag{9.34}$$

where again

$$\boldsymbol{\beta}_0=E\left\{\bar{\boldsymbol{\beta}}\right\}=\tilde{\boldsymbol{B}}^{\mathrm{T}}\boldsymbol{G}\,\boldsymbol{x}_{\mathbf{0}}$$

is taken for granted. Referring to a weight matrix of the form

$$\boldsymbol{G}=\left[E\left\{\left(\bar{\boldsymbol{x}}-\boldsymbol{x}_0\right)\left(\bar{\boldsymbol{x}}-\boldsymbol{x}_0\right)^{\mathrm{T}}\right\}\right]^{-1/2}\,, \tag{9.35}$$

the theoretical variance–covariance matrix of the weighted ISO adjustment is given by

$$\begin{aligned}E\left\{\left(\bar{\boldsymbol{\beta}}-\boldsymbol{\beta}_0\right)\left(\bar{\boldsymbol{\beta}}-\boldsymbol{\beta}_0\right)^{\mathrm{T}}\right\}&=\tilde{\boldsymbol{B}}^{\mathrm{T}}\boldsymbol{G}E\left\{\left(\bar{\boldsymbol{x}}-\boldsymbol{x}_0\right)\left(\bar{\boldsymbol{x}}-\boldsymbol{x}_0\right)^{\mathrm{T}}\right\}\boldsymbol{G}\tilde{\boldsymbol{B}}\\&=\tilde{\boldsymbol{B}}^{\mathrm{T}}\tilde{\boldsymbol{B}}=\left[\left(\boldsymbol{G}\boldsymbol{A}\right)^{\mathrm{T}}\left(\boldsymbol{G}\boldsymbol{A}\right)\right]^{-1}\,.\end{aligned} \tag{9.36}$$

Again, the square roots of the diagonal elements of this matrix act as the uncertainties of the weighted adjustment.

Let us recall, on account of the randomization postulate, there is no distinction between the expectation $E\left\{\bar{\boldsymbol{\beta}}\right\}$ of the estimator $\bar{\boldsymbol{\beta}}$ and its true value $\boldsymbol{\beta}_0$. According to (9.21) and (9.22), however, these quantities differ by the biases

$$\boldsymbol{B}^{\mathrm{T}}\boldsymbol{f}\quad\text{and}\quad\tilde{\boldsymbol{B}}^{\mathrm{T}}\boldsymbol{G}\boldsymbol{f}$$

respectively. After all, the experimenter has no means to exclude the possibility that the weights have shifted his estimators away from their true values and, paradoxically, shrunk their uncertainties.

Examples

(i) Non-weighted and weighted adjustment: A computer simulation shall help us to compare the error model of the *ISO Guide* with that of the alternative approach. To this end we consider the linear system

$$\begin{aligned}10\,\beta_1+\;\;\beta_2+9\,\beta_3&\approx\bar{x}_1\\-\,\beta_1\qquad\quad+2\,\beta_3&\approx\bar{x}_2\\\beta_1+2\,\beta_2+3\,\beta_3&\approx\bar{x}_3\\-3\,\beta_1-\;\;\beta_2+2\,\beta_3&\approx\bar{x}_4\\\beta_1+2\,\beta_2+\;\;\beta_3&\approx\bar{x}_5\end{aligned}$$

and let

$$\beta_{0,1} = 1\,, \quad \beta_{0,2} = 2\,, \quad \beta_{0,3} = 3$$

be the true values of the parameters so that the true values of the input data turn out to be

$$x_{0,1} = 39\,, \quad x_{0,2} = 5\,, \quad x_{0,3} = 14\,, \quad x_{0,4} = 1\,, \quad x_{0,5} = 8\,.$$

We simulate normally distributed input data x_{il}; $i = 1, \ldots, 5$; $l = 1, \ldots, 10$. It seems recommendable to process random and systematic errors of the same order of magnitude. That's why we set, for any fixed i, the theoretical variance of the random errors equal to the postulated theoretical variance of the pertaining f_i,

$$\sigma_{x_i}^2 = \frac{1}{3} f_{s,i}^2\,; \quad i = 1\,, \ldots,\, m\,.$$

We assume the boundaries of the systematic errors and their actual values to be

$$\begin{aligned} f_{s,1} &= 0.39 \times 10^{-2}\,, \quad f_{s,2} = 0.35 \times 10^{-4}\,, \quad f_{s,3} = 0.98 \times 10^{-5} \\ f_{s,4} &= 0.35 \times 10^{-4}\,, \quad f_{s,5} = 0.8 \times 10^{-3} \end{aligned}$$

and

$$\begin{aligned} f_1 &= 0.351 \times 10^{-2}\,, \quad f_2 = 0.315 \times 10^{-4}\,, \quad f_3 = -0.882 \times 10^{-5} \\ f_4 &= -0.315 \times 10^{-4}\,, \quad f_5 = -0.72 \times 10^{-3} \end{aligned}$$

respectively, i.e. we multiplied the boundaries $f_{s,i}$; $i = 1, \ldots, 5$ by a factor of 0.9 and purposefully chose the signs of the actual systematic errors in such a way that the *Guide's* 2σ uncertainties of the weighted adjustment fail to localize the true values $\beta_{0,k}$ of the estimators $\bar{\beta}_k$.

We refer to a weight matrix $\boldsymbol{G}$ of the form (8.35), the entries being the reciprocals of the uncertainties of the input data corresponding to the *ISO Guide* and to the alternative approach respectively, i.e.

$$g_i = 1/u_{\bar{x}_i}\,, \quad i = 1, \ldots, 5$$

with

$$u_{\bar{x}_i} = \sqrt{\frac{s_{x_i}^2}{n} + \frac{1}{3} f_{s,i}^2} \quad \textit{ISO Guide} \quad \text{and}$$

$$u_{\bar{x}_i} = \frac{t_P(n-1)}{\sqrt{n}} s_{x_i} + f_{s,i} \quad \text{alternative model}\,.$$

The alternative error model allows us to manipulate the weights of the adjustment. To exemplify this possibility we choose

$$g_1 = 1/u_{\bar{x}_1} \quad g_2 = 4/u_{\bar{x}_2} \quad g_3 = 10/u_{\bar{x}_3} \quad g_4 = 4/u_{\bar{x}_4} \quad g_5 = 1/u_{\bar{x}_5}\,.$$

For the *ISO Guide* we quote so-called 2σ uncertainties. The alternative error model relates the random parts of the overall uncertainties to a confidence level of $P = 95\%$.

Tables 9.1–9.3 display the results. In general, the 2σ uncertainties of the *Guide* may be considered acceptable. There are, however, singular cases in which the *Guide* fails to localize the true values of the estimators. We purposefully exemplified this situation thus underscoring that the *Guide's* 2σ uncertainties can be too short.

In contrast to this, the alternative approach presents us with robust uncertainties safely localizing the true values of the estimators. Even if we manipulate the weights, the localization property of the alternative error model still persists.

(ii) Weighted mean of means: Given m arithmetic means and their respective uncertainties,

$$\bar{x}_i = \frac{1}{n}\sum_{l=1}^{n} x_{il}\,; \quad u_{\bar{x}_i} = \frac{t_P\,(n-1)}{\sqrt{n}} s_i + f_{s,i}\,; \quad i = 1\,, \ldots,\, m\,. \tag{9.37}$$

We shall find the weighted grand mean $\bar{\beta}$ and its uncertainty $u_{\bar{\beta}}$.

To average a pool of given arithmetic means ranks among the most frequently used standard procedures of metrology. Clearly, this is done in order to extract as much information as possible out of the data. The proceeding is taken permissible, trouble-free and self-evident. But consider the following proposal:

Averaging a set of means makes sense only if the underlying true values $x_{0,i}$; $i = 1, \ldots, m$ are *identical.*

As has been discussed in Sect. 7.1, to average means to perform a least squares adjustment. Here we have, instead of (7.2),

Table 9.1. Least squares estimators and their uncertainties based on the *ISO Guide* and the alternative error model, respectively. In the first case so-called 2σ uncertainties have been quoted, in the latter case the random parts of the overall uncertainties refer to a confidence level of P=95%. The * notifies manipulated weights

Model	$\bar{\beta}_1 \pm u_{\bar{\beta}_1}$	$\bar{\beta}_2 \pm u_{\bar{\beta}_2}$	$\bar{\beta}_3 \pm u_{\bar{\beta}_3}$
ISO non-weighted	1.0003 ± 0.0004	1.9995 ± 0.0005	3.00016 ± 0.00021
ISO weighted	1.00013 ± 0.00011	1.99980 ± 0.00016	3.00009 ± 0.00007
altern. non-weighted	1.0003 ± 0.0005	1.9995 ± 0.0008	3.00017 ± 0.00029
altern. weighted	1.00014 ± 0.00020	1.99978 ± 0.00030	3.00009 ± 0.00013
altern. weighted*	1.00012 ± 0.00017	1.99981 ± 0.00025	3.00008 ± 0.00011

Table 9.2. Data taken from Table 9.1: Localization in least squares adjustment based on the *ISO Guide*. The weighted adjustment fails to localize the true values

ISO Guide	
non-weighted	weighted
$0.9999 < 1 < 1.0007$	$1.00002 > 1 < 1.00024$
$1.9990 < 2 = 2.0000$	$1.99964 < 2 > 1.99996$
$2.99995 < 3 < 3.00037$	$3.00002 > 3 < 3.00016$

Table 9.3. Data taken from Table 9.1: Localization in least squares adjustmentvbased on the alternative error model. The * notifies manipulated weights

alternative model		
non-weighted	weighted	weighted*
$0.9998 < 1 < 1.0008$	$0.99994 < 1 < 1.00034$	$0.99995 < 1 < 1.00029$
$1.9987 < 2 < 2.0003$	$1.99948 < 2 < 2.00008$	$1.99956 < 2 < 2.00006$
$2.99988 < 3 < 3.00046$	$2.99996 < 3 < 3.00022$	$2.99997 < 3 < 3.00019$

$$\begin{pmatrix} 1 \\ 1 \\ \dots \\ 1 \end{pmatrix} \beta \approx \begin{pmatrix} \bar{x}_1 \\ \bar{x}_2 \\ \dots \\ \bar{x}_m \end{pmatrix}, \quad \text{i.e.} \quad \boldsymbol{a}\beta \approx \bar{\boldsymbol{x}}\,. \tag{9.38}$$

Obviously, the underlying consistent system reads

$$\begin{pmatrix} 1 \\ 1 \\ \dots \\ 1 \end{pmatrix} \beta_0 = \begin{pmatrix} x_{0,1} \\ x_{0,2} \\ \dots \\ x_{0,m} \end{pmatrix}. \tag{9.39}$$

From this we take that the true value β_0 of the grand mean $\bar{\beta}$ cannot comply with different true values of the input data. Consequently we have to require identical true values $x_{0,i} = x_0$; $i = 1, \dots, m$.

Nevertheless, we might wish to average "ad hoc", i.e. without resorting to the method of least squares. Let us average two masses $m_1 = 1/4\,\mathrm{kg}$ and $m_2 = 3/4\,\mathrm{kg}$ each being accurate to about $\pm 1\,\mathrm{mg}$ each. The mean is $\bar{m} = 1/2\,\mathrm{kg}$. However, the associated uncertainty exceeds the uncertainties of the input data by the factor 250 000. The uncertainty has been blown up since the true values of the masses differ. We are sure, uncertainties should be due to measurement errors and not to deviant true values. This drastically exaggerating example elucidates that the averaging of means implies far-reaching consequences if done inappropriately.

To weight the inconsistent linear system

$$\boldsymbol{a}\beta \approx \bar{\boldsymbol{x}}$$

we set

$$\boldsymbol{G} = \operatorname{diag}\{g_1\,,\quad g_2\,,\quad \ldots\,,\quad g_m\}\;;\quad g_i = 1/u_{\bar{x}_i}$$

so that

$$\boldsymbol{G}\boldsymbol{a}\beta \approx \boldsymbol{G}\bar{\boldsymbol{x}}. \tag{9.40}$$

The least squares estimator is

$$\bar{\beta} = \sum_{i=1}^{m} w_i \bar{x}_i\,;\quad w_i = \frac{g_i^2}{\sum\limits_{i=1}^{m} g_i^2}\,. \tag{9.41}$$

Let us replace the means $\bar{x}_1, \bar{x}_2, \ldots, \bar{x}_m$ with the respective l-th individual measurements $x_{1l}, x_{2l}, \ldots, x_{ml}$

$$\begin{array}{llllllllll} x_{11} & x_{12} & \ldots & x_{1l} & \ldots & x_{1n} & \Rightarrow & \bar{x}_1 \\ x_{21} & x_{22} & \ldots & x_{2l} & \ldots & x_{2n} & \Rightarrow & \bar{x}_2 \\ \ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots \\ x_{m1} & x_{m2} & \ldots & x_{ml} & \ldots & x_{ml} & \Rightarrow & \bar{x}_m\,. \end{array} \tag{9.42}$$

Then, (9.41) turns into

$$\bar{\beta}_l = \sum_{i=1}^{m} w_i x_{il}\,;\quad l = 1\,, \ldots,\, n \tag{9.43}$$

so that

$$\bar{\beta} = \frac{1}{n}\sum_{l=1}^{n} \bar{\beta}_l\,. \tag{9.44}$$

Inserting

$$x_{il} = x_{0,i} + (x_{il} - \mu_i) + f_i\,;\quad \bar{x}_i = x_{0,i} + (\bar{x}_i - \mu_i) + f_i\,,$$

(9.41) and (9.43) yield

$$\begin{aligned} \bar{\beta}_l &= \sum_{i=1}^{m} w_i\,[x_{0,i} + (x_{il} - \mu_i) + f_i] \quad \text{and} \\ \bar{\beta} &= \sum_{i=1}^{m} w_i\,[x_{0,i} + (\bar{x}_i - \mu_i) + f_i]\,. \end{aligned} \tag{9.45}$$

Being free from systematic errors, the difference

$$\bar{\beta}_l - \bar{\beta} = \sum_{i=1}^{m} w_i \left(x_{il} - \bar{x}_i\right) \tag{9.46}$$

solely expresses the influence of random errors. Consequently, the empirical variance of the estimator $\bar{\beta}$ is given by

$$\begin{aligned} s_{\bar{\beta}}^2 &= \frac{1}{n-1} \sum_{l=1}^{n} \left(\bar{\beta}_l - \bar{\beta}\right)^2 \\ &= \frac{1}{n-1} \sum_{l=1}^{n} \left[\sum_{i=1}^{m} w_i \left(x_{il} - \bar{x}_i\right)\right] \left[\sum_{j=1}^{m} w_j \left(x_{jl} - \bar{x}_j\right)\right] \\ &= \sum_{i,j}^{m} w_i w_j s_{ij} \end{aligned} \tag{9.47}$$

where the

$$s_{ij} = \frac{1}{n-1} \sum_{l=1}^{n} \left(x_{il} - \bar{x}_i\right)\left(x_{jl} - \bar{x}_j\right) \; ; \quad i,j = 1,\ldots,m \, ; \quad s_{ii} \equiv s_i^2 \tag{9.48}$$

denote the empirical variances and covariances of the input data (9.42). Again, the s_{ij} shall define the empirical variance–covariance matrix $\boldsymbol{s}$ and the weights w_i an auxiliary vector $\boldsymbol{w}$,

$$\boldsymbol{s} = \begin{pmatrix} s_{11} & s_{12} & \ldots & s_{1m} \\ s_{21} & s_{22} & \ldots & s_{2m} \\ \ldots & \ldots & \ldots & \ldots \\ s_{m1} & s_{m2} & \ldots & s_{mm} \end{pmatrix} \; ; \quad \boldsymbol{w} = \begin{pmatrix} w_1 & w_2 & \cdots & w_m \end{pmatrix}^{\mathrm{T}} .$$

Hence, (9.47) takes the form

$$s_{\bar{\beta}}^2 = \boldsymbol{w}^{\mathrm{T}} \boldsymbol{s}\, \boldsymbol{w} \, . \tag{9.49}$$

The propagated systematic errors follow from (9.45),

$$f_{\bar{\beta}} = \sum_{i=1}^{m} w_i f_i \, ,$$

and its worst case estimation is

$$f_{s,\bar{\beta}} = \sum_{i=1}^{m} w_i f_{s,i} \, . \tag{9.50}$$

Let us formally assign an m-dimensional normal density to each of the n data sets

$$x_{1l}, x_{2l}, \ldots, x_{ml}\,; \quad l = 1, \ldots, n \tag{9.51}$$

depicted as columns in the decomposition (9.42). But then the $\bar{\beta}_l$; $l = 1, \ldots, n$ given in (9.43) are normally distributed – whether there are dependencies between the individuals $x_{1l}, x_{2l}, \ldots, x_{ml}$, l fixed, remains immaterial. Moreover, as we consider the n successive sets (9.51) to be independent, the $\bar{\beta}_l$ are also independent.

Finally, the overall uncertainty of the weighted mean $\bar{\beta}$ is given by

$$u_{\bar{\beta}} = \frac{t_P}{\sqrt{n}} \sqrt{\sum_{i,j}^{m} w_i w_j s_{ij}} + \sum_{i=1}^{m} w_i f_{s,i}\,. \tag{9.52}$$

It looks as if (9.50) would overestimate the influence of systematic errors, i.e. as if $f_{s,\bar{\beta}}$ might grow inadequately, the greater the number m of input data. This is not, however, the case, as the following two examples suggest.

Given $u_{\bar{x}_1} = u_{\bar{x}_2} = u_{\bar{x}_3}$, we find $w_1 = w_2 = w_3 = 1/3$ so that

$$f_{s,\,\bar{\beta}} = (f_{s,\,1} + f_{s,\,2} + f_{s,\,3})\,/3\,.$$

Given $u_{\bar{x}_1} = a$, $u_{\bar{x}_2} = 2a$, $u_{\bar{x}_3} = 3a$ we obtain $w_1 = 36/49$, $w_2 = 9/49$, $w_1 = 4/49$, i.e.

$$f_{s,\,\bar{\beta}} = (36 f_{s,\,1} + 9 f_{s,\,2} + 4 f_{s,\,3})\,/49\,.$$

Due to the weight factors w_i, the propagated systematic error preserves quite a reasonable order of magnitude even if the number of means entering the average should be large.

Let us summarize: We conclude that the *Guide's* recommendation to assign distribution densities to unknown systematic errors should scarcely be tenable.

Over the years, appreciable efforts have been undertaken to develop a formalism allowing experimenters to randomize detected unknown systematic errors and to somehow repair the bothersome observation (8.57).

Ultimately, the inconsistencies in meeting the influence of unknown systematic errors had condensed themselves into a sheerly inextricable clew of different procedures competing with one another, similar to a Gordian knot. In connection with the adjustment of the fundamental constants of physics, even the abolition of the method of least squares was discussed [13].

Arguably, the idea of treating unknown systematic errors on a probabilistic basis was inspired by the objective of designing lowest possible measurement uncertainties. The analysis of variance disclosed, however, a first inconsistency, Sect. 4.3. The computer simulations testing the reliability of the *Guide's* measurement uncertainties showed that there are situations in which even so-called 2σ uncertainties turn out to be too small, Sect. 6.4. The task to calculate the grand mean of a group of means accentuated anew

the need to base data evaluations on true values, Sect. 9.3. Finally, as (8.57) underscored, (8.56) seems to reflect the actual metrological situation more realistically than (8.55) could.

On the other hand, we are in a position to undo the Gordian knot as soon as we are willing to abstain from randomizing systematic errors. Then, we understand why the standard tools of data evaluation do no longer produce reasonable results, applied to data of empirical origin. It suggests that we either revise those classical concepts according to the prevailing metrological situation, or, if necessary, abolish them. Only then shall we be in a position to interlace our measurement results within a reliable and traceable metrological net of data.

Though a rigorous revision of the error calculus might appear uninviting, above all the aim is to extract a maximum of reliable, objectively justifiable information out of the measurements which, as is well known, require considerable efforts even in standard cases and virtually huge efforts in special cases.[2]

9.4 Uncertainty of a Function of Estimators

According to Sect. 6.5, we shall quote the uncertainty $u_{\bar\phi}$ of a given function ϕ of the components $\bar\beta_1, \bar\beta_2, \ldots, \bar\beta_r$ of the least squares estimator $\bar{\boldsymbol{\beta}}$, i.e. we shall look for

$$\bar\beta_1 \pm u_{\bar\beta_1},\ \bar\beta_2 \pm u_{\bar\beta_2},\ \ldots,\ \bar\beta_r \pm u_{\bar\beta_r} \quad \Rightarrow \quad \phi\left(\bar\beta_1, \bar\beta_2, \ldots, \bar\beta_r\right) \pm u_{\bar\phi}\,. \tag{9.53}$$

For simplicity, we confine ourselves to a function of two estimators $\bar\beta_1, \bar\beta_2$ and, as usual, neglect the errors of the linearization of ϕ. Inserting

$$\bar x_i = x_{0,i} + (\bar x_i - \mu_i) + f_i\,; \quad i = 1, \ldots, m$$

into

$$\bar\beta_1 = \sum_{i=1}^{m} b_{i1}\bar x_i \quad \text{and} \quad \bar\beta_2 = \sum_{i=1}^{m} b_{i2}\bar x_i$$

yields

$$\bar\beta_k = \beta_{0,k} + \sum_{i=1}^{m} b_{ik}\,(\bar x_i - \mu_i) + \sum_{i=1}^{m} b_{ik} f_i\,; \quad k = 1, 2$$

so that

[2] The vacuum tube of the Large Hadron Collider (LHC) of the European Organization for Nuclear Research (CERN), Geneva has a circumference of 27 km, and its magnets work near absolute zero. Among the results physicists are waiting for is the proof of the Higgs boson.

$$\phi\left(\bar{\beta}_1,\bar{\beta}_2\right)=\phi\left(\beta_{0,1},\beta_{0,2}\right)+\frac{\partial\phi}{\partial\bar{\beta}_1}\left[\sum_{i=1}^{m}b_{i1}\left(\bar{x}_i-\mu_i\right)\right]+\frac{\partial\phi}{\partial\bar{\beta}_2}\left[\sum_{i=1}^{m}b_{i2}\left(\bar{x}_i-\mu_i\right)\right]$$
$$+\frac{\partial\phi}{\partial\bar{\beta}_1}\left[\sum_{i=1}^{m}b_{i1}f_i\right]+\frac{\partial\phi}{\partial\bar{\beta}_2}\left[\sum_{i=1}^{m}b_{i2}f_i\right]$$

or

$$\phi\left(\bar{\beta}_1,\bar{\beta}_2\right)=\phi\left(\beta_{0,1},\beta_{0,2}\right)+\sum_{i=1}^{m}\left(\frac{\partial\phi}{\partial\bar{\beta}_1}b_{i1}+\frac{\partial\phi}{\partial\bar{\beta}_2}b_{i2}\right)\left(\bar{x}_i-\mu_i\right)$$
$$+\sum_{i=1}^{m}\left(\frac{\partial\phi}{\partial\bar{\beta}_1}b_{i1}+\frac{\partial\phi}{\partial\bar{\beta}_2}b_{i2}\right)f_i\,. \tag{9.54}$$

To abbreviate, we put

$$\chi_i=\frac{\partial\phi}{\partial\bar{\beta}_1}\,b_{i1}+\frac{\partial\phi}{\partial\bar{\beta}_2}\,b_{i2}\,;\quad i=1,\ldots,m\,. \tag{9.55}$$

Then, (9.54) turns into

$$\phi\left(\bar{\beta}_1,\bar{\beta}_2\right)=\phi\left(\beta_{0,1},\beta_{0,2}\right)+\sum_{i=1}^{m}\chi_i\left(\bar{x}_i-\mu_i\right)+\sum_{i=1}^{m}\chi_i f_i\,. \tag{9.56}$$

For convenience, we also assign the χ_i; $i=1,\ldots,m$ to an $(m\times 1)$ column vector

$$\boldsymbol{\chi}=\left(\chi_1\quad\chi_2\quad\ldots\quad\chi_m\right)^{\mathrm{T}}\,. \tag{9.57}$$

First, we assess the second term on the right hand side of (9.56), which, apparently, is due to random errors. With reference to the notations (9.2), (9.3) and (9.4),

$$\bar{\beta}_k=\sum_{i=1}^{m}b_{ik}\bar{x}_i=\frac{1}{n}\sum_{l=1}^{n}\bar{\beta}_{kl}\,;\quad\bar{\beta}_{kl}=\sum_{i=1}^{m}b_{ik}x_{il}\,;\quad k=1,2\,,$$

we expand $\phi(\bar{\beta}_{1l},\bar{\beta}_{2l})$ throughout a neighborhood of $\bar{\beta}_1,\bar{\beta}_2$,

$$\begin{aligned}\phi\left(\bar{\beta}_{1l},\bar{\beta}_{2l}\right)&=\phi\left(\bar{\beta}_1,\bar{\beta}_2\right)+\frac{\partial\phi}{\partial\bar{\beta}_1}\left(\bar{\beta}_{1l}-\bar{\beta}_1\right)+\frac{\partial\phi}{\partial\bar{\beta}_2}\left(\bar{\beta}_{2l}-\bar{\beta}_2\right)\\&=\phi\left(\bar{\beta}_1,\bar{\beta}_2\right)+\sum_{i=1}^{m}\left(\frac{\partial\phi}{\partial\bar{\beta}_1}\,b_{i1}+\frac{\partial\phi}{\partial\bar{\beta}_2}\,b_{i2}\right)\left(x_{il}-\bar{x}_i\right)\\&=\phi\left(\bar{\beta}_1,\bar{\beta}_2\right)+\sum_{i=1}^{m}\chi_i\left(x_{il}-\bar{x}_i\right).\end{aligned}$$

The difference $\phi(\bar{\beta}_{1l},\bar{\beta}_{2l})-\phi(\bar{\beta}_1,\bar{\beta}_2)$ leads us to the empirical variance

$$s^2_{\bar\phi} = \frac{1}{n-1}\sum_{l=1}^{n}\left[\phi\left(\bar\beta_{1l},\bar\beta_{2l}\right) - \phi\left(\bar\beta_1,\bar\beta_2\right)\right]^2 = \boldsymbol{\chi}^{\mathrm{T}}\boldsymbol{s}\,\boldsymbol{\chi}\,. \tag{9.58}$$

Here, $\boldsymbol{s}$ designates the empirical variance–covariance matrix of the input data (9.9) and the vector $\boldsymbol{\chi}$ has been defined in (9.57).

The third term on the right of (9.56),

$$f_{\bar\phi} = \sum_{i=1}^{m}\chi_i f_i\,, \tag{9.59}$$

is due to the propagation of systematic errors. Its worst case estimation yields

$$f_{s,\bar\phi} = \sum_{i=1}^{m}|\chi_i| f_{s,i}\,. \tag{9.60}$$

Finally, the overall uncertainty of the estimator $\phi(\bar\beta_1,\bar\beta_2)$ turns out to be

$$u_{\bar\phi} = \frac{t_P\,(n-1)}{\sqrt{n}}\sqrt{\boldsymbol{\chi}^{\mathrm{T}}\boldsymbol{s}\,\boldsymbol{\chi}} + \sum_{i=1}^{m}|\chi_i| f_{s,i}\,. \tag{9.61}$$

Before any particular worst case estimate can be carried out, we have to merge in brackets all terms relating to the same f_i, otherwise the triangle inequality would overestimate the share of the overall uncertainty cause by systematic errors.

9.5 Uncertainty Spaces

The preceding section dwelled on the problem of how to estimate the uncertainty $u_{\bar\phi}$ of a given function ϕ, linking some or all of the least squares estimators. Now we turn toward the problem of spanning so-called uncertainty spaces by means of the estimators themselves.

Let us illustrate this notion by conceiving a least squares adjustment to a circle. Should it suffice to estimate just the radius r, we can confine ourselves to a result of the form $\bar r \pm u_{\bar r}$. However, if we additionally want to know all about where we may insert the tip of the compasses and how wide to open its legs, we have to revert to the couplings between the radius r and the coordinates x_M, y_M of its center hidden within the adjustment's quotations

$$\bar x_M \pm u_{\bar x_M}\,, \quad \bar y_M \pm u_{\bar y_M}\,; \quad \bar r \pm u_{\bar r}\,.$$

These intervals obviously imply all circles which are compatible with the input data and the error model. We expect the latter to provide a small circular region localizing the true center x_0, y_0 of the circle and a large annular region enclosing the true arc $x_0, y_0; r_0$. We shall treat this problem in Sect. 11.4.

The origin of the couplings between the components of the estimator $\bar{\boldsymbol{\beta}}$ is obvious. As each of the r components

$$\begin{aligned}\bar{\beta}_k &= \sum_{i=1}^{m} b_{ik}\bar{x}_i \\ &= \beta_{0,k} + \sum_{i=1}^{m} b_{ik}\,(\bar{x}_i - \mu_i) + \sum_{i=1}^{m} b_{ik} f_i\,; \quad k = 1, \ldots, r \end{aligned} \tag{9.62}$$

relies on one and the same set of input data, the $\bar{\beta}_k$ are necessarily dependent. The second term on the right-hand side expresses the couplings due to random errors. As the $\bar{x}_i$ imply the same number of repeat measurements, we gain access to the complete empirical variance–covariance matrix of the input data. Hence, we are in a position to formalize the said dependencies by Hotelling's density. Remarkably enough, the confidence ellipsoids provided by this density differ substantially from those referred to in the conventional error calculus. As is known, the conventional error calculus obtains its confidence ellipsoids from the exponent of the multidimensional normal probability density so that they are based on unknown theoretical variances and covariances, thus hampering metrological interpretations.

Finally, the third term on the right-hand side of (9.62) formalizes the couplings due to systematic errors, i.e. to influences entirely ignored on the part of the Gaussian error calculus.

9.5.1 Confidence Ellipsoids

Let us reconsider the decomposition (9.3),

$$\bar{\beta}_k = \frac{1}{n}\sum_{l=1}^{n} \bar{\beta}_{kl}\,; \quad k = 1, \ldots, r$$

where, as (9.4) shows,

$$\bar{\beta}_{kl} = \sum_{i=1}^{m} b_{ik} x_{il}\,; \quad k = 1, \ldots, r, \quad l = 1, \ldots, n\,.$$

Assuming normally distributed measured values x_{il}, the $\bar{\beta}_{kl}$ are also normally distributed, furthermore, as has already been discussed, they are independent. The empirical variance–covariance matrix of the $\bar{\beta}_k$ has been stated in (9.12),

$$\boldsymbol{s}_{\bar{\beta}} = \boldsymbol{B}^{\mathrm{T}} \boldsymbol{s}\, \boldsymbol{B}\,.$$

To establish Hotelling's ellipsoid, we refer to (3.73).[3] Assembling the expectations

[3] I am grateful to Dr. Wöger for calling my attention to this analogy.

$$\mu_{\bar{\beta}_k} = E\left\{\bar{\beta}_k\right\} = \beta_{0,k} + \sum_{i=1}^{m} b_{ik} f_i\,; \quad k = 1, \ldots, r \tag{9.63}$$

within a column vector $\boldsymbol{\mu}_{\bar{\boldsymbol{\beta}}}$ as we did in (8.8), we have

$$t_P^2\,(r,n) = n\left(\bar{\boldsymbol{\beta}} - \boldsymbol{\mu}_{\bar{\beta}}\right)^{\mathrm{T}} \left(\boldsymbol{B}^{\mathrm{T}} \boldsymbol{s}\, \boldsymbol{B}\right)^{-1} \left(\bar{\boldsymbol{\beta}} - \boldsymbol{\mu}_{\bar{\beta}}\right)\,. \tag{9.64}$$

The ellipsoid is centered in $\boldsymbol{\mu}_{\bar{\boldsymbol{\beta}}}$; the probability of holding any realization of $\bar{\boldsymbol{\beta}}$ is given by

$$P = \int_0^{t_P(r,n)} p_T\,(t; r, n)\, dt\,; \tag{9.65}$$

$p_T(t; r, n)$ has been stated in (3.75). Experimentally speaking, the vector $\boldsymbol{\mu}_{\bar{\boldsymbol{\beta}}}$ cannot be known. On the other hand, we may refer (9.64) to $\bar{\boldsymbol{\beta}}$ and substitute an auxiliary vector $\boldsymbol{\beta}$ for $\boldsymbol{\mu}_{\bar{\boldsymbol{\beta}}}$. The so-defined confidence ellipsoid

$$\frac{t_P^2\,(r,n)}{n} = \left(\boldsymbol{\beta} - \bar{\boldsymbol{\beta}}\right)^{\mathrm{T}} \left(\boldsymbol{B}^{\mathrm{T}} \boldsymbol{s}\, \boldsymbol{B}\right)^{-1} \left(\boldsymbol{\beta} - \bar{\boldsymbol{\beta}}\right) \tag{9.66}$$

localizes the vector $\boldsymbol{\mu}_{\bar{\boldsymbol{\beta}}}$ with probability P as given in (9.65). In principle, this procedure is similar to that we have used to define one-dimensional confidence intervals in Sect. 5.1.

9.5.2 The New Solids

The propagated systematic errors define a geometric solid as well. According to (9.62), it is constituted by the components

$$f_{\bar{\beta}_k} = \sum_{i=1}^{m} b_{ik} f_i\,; \quad -f_{s,i} \le f_i \le f_{s,i}\,; \quad k = 1, \ldots, r \tag{9.67}$$

of the vector

$$\boldsymbol{f}_{\bar{\boldsymbol{\beta}}} = \boldsymbol{B}^{\mathrm{T}} \boldsymbol{f} = \begin{pmatrix} f_{\bar{\beta}_1} & f_{\bar{\beta}_2} & \cdots & f_{\bar{\beta}_r} \end{pmatrix}^{\mathrm{T}}\,. \tag{9.68}$$

In a sense, the solid comes into being by letting the vector

$$\boldsymbol{f} = \begin{pmatrix} f_1 & f_2 & \cdots & f_m \end{pmatrix} \tag{9.69}$$

"scan" the set of points defined by the m-dimensional hypercuboid

$$-f_{s,i} \le f_i \le f_{s,i}\,; \quad i = 1, 2, \ldots, m \tag{9.70}$$

and lying within and on its boundary surfaces. It goes without saying that all vectors $\boldsymbol{f}$ of the null space $N(\boldsymbol{B}^{\mathrm{T}})$ of the matrix $\boldsymbol{B}^{\mathrm{T}}$ are mapped into the null vector $\boldsymbol{f}_{\bar{\boldsymbol{\beta}}} = 0$ and will not be of interest to us.

To begin with, let us focus on some fundamental properties of the linear singular mapping (9.67). The projected solid is

– enclosed within an r-dimensional hypercuboid of extensions

$$-f_{s,\bar{\beta}_k} \le f_{\bar{\beta}_k} \le f_{s,\bar{\beta}_k}\,; \quad f_{s,\bar{\beta}_k} = \sum_{i=1}^{m} |b_{ik}|\, f_{s,i}\,; \quad k = 1, 2, \ldots, r \tag{9.71}$$

– convex, as the mapping is linear and the hypercuboid (9.70) is convex.[4] For any $\tau \in [0, 1]$ we have

$$\boldsymbol{f}_{\bar{\boldsymbol{\beta}}} = \boldsymbol{f}^{(1)}_{\bar{\boldsymbol{\beta}}} + \tau \left(\boldsymbol{f}^{(2)}_{\bar{\boldsymbol{\beta}}} - \boldsymbol{f}^{(1)}_{\bar{\boldsymbol{\beta}}} \right) = \boldsymbol{B}^{\mathrm{T}} \left[\boldsymbol{f}_1 + \tau \left(\boldsymbol{f}_2 - \boldsymbol{f}_1 \right) \right] ,$$

as every point on the line connecting any two vectors $\boldsymbol{f}_1$ and $\boldsymbol{f}_2$ is a point of the hypercuboid (9.70), all points on the line connecting the vectors $\boldsymbol{f}^{(1)}_{\bar{\boldsymbol{\beta}}}$ and $\boldsymbol{f}^{(2)}_{\bar{\boldsymbol{\beta}}}$ are points of the (yet unknown) solid (9.67)

– point-symmetric, as for any vector $\hat{\boldsymbol{f}} = -\boldsymbol{f}$ there is a vector $\hat{\boldsymbol{f}}_{\bar{\boldsymbol{\beta}}} = -\boldsymbol{f}_{\bar{\boldsymbol{\beta}}}$.

As we shall see, the objects in question are polygons in case of two measurands, polyhedra in case of three and abstract polytopes if there are more than three measurands. Moreover, we suggest to add the prefix security, i.e. to speak of security polygons, security polyhedra and security polytopes. In a sense, this naming would correspond to the terms confidence ellipses and confidence ellipsoids.

Security Polygons

In the first instance, we shall confine ourselves to couplings between just two propagated systematic errors, $f_{\bar{\beta}_k}$; $k = 1, 2$. Assuming $m = 5$, we have

$$\begin{aligned} f_{\bar{\beta}_1} &= b_{11} f_1 + b_{21} f_2 + b_{31} f_3 + b_{41} f_4 + b_{51} f_5 \\ f_{\bar{\beta}_2} &= b_{12} f_1 + b_{22} f_2 + b_{32} f_3 + b_{42} f_4 + b_{52} f_5 \,, \end{aligned} \tag{9.72}$$

where

$$-f_{s,i} \le f_i \le f_{s,i}\,; \quad i = 1, \ldots, 5\,. \tag{9.73}$$

Let us refer to a rectangular $f_{\bar{\beta}_1}, f_{\bar{\beta}_2}$ coordinate system. According to (9.71), the geometrical figure in question will be enclosed within a rectangle

$$-f_{s,\bar{\beta}_1}, \ldots, f_{s,\bar{\beta}_1}\,; \quad -f_{s,\bar{\beta}_2}, \ldots, f_{s,\bar{\beta}_2}\,.$$

Let $b_{11} \neq 0$. Eliminating f_1, we arrive at a straight line,

$$f_{\bar{\beta}_2} = \frac{b_{12}}{b_{11}} f_{\bar{\beta}_1} + c_1 \,, \tag{9.74}$$

[4] Imagine a straight line connecting any two points of a given solid. If every point on the line is a point of the solid, the latter is called convex. There will then be neither hollows inside the solid nor folds in its hull.

where

$$c_1 = h_{12} f_2 + h_{13} f_3 + h_{14} f_4 + h_{15} f_5$$

and

$$h_{12} = \frac{1}{b_{11}} \left(b_{11} b_{22} - b_{12} b_{21} \right) , \quad h_{13} = \frac{1}{b_{11}} \left(b_{11} b_{32} - b_{12} b_{31} \right) ,$$
$$h_{14} = \frac{1}{b_{11}} \left(b_{11} b_{42} - b_{12} b_{41} \right) , \quad h_{15} = \frac{1}{b_{11}} \left(b_{11} b_{52} - b_{12} b_{51} \right) .$$

Any variation of c_1 shifts the line (9.74) parallel to itself; c_1 is maximal if

$$f_2 = f_2^* = \operatorname{sign}(h_{12})\, f_{s,2} , \quad f_3 = f_3^* = \operatorname{sign}(h_{13})\, f_{s,3} ,$$
$$f_4 = f_4^* = \operatorname{sign}(h_{14})\, f_{s,4} , \quad f_5 = f_5^* = \operatorname{sign}(h_{15})\, f_{s,5} . \tag{9.75}$$

But then

$$c_{s,1} = h_{12} f_2^* + h_{13} f_3^* + h_{14} f_4^* + h_{15} f_5^*$$

and

$$-c_{s,1} \le c_1 \le c_{s,1} . \tag{9.76}$$

Of all the lines specified in (9.74), the lines

$$f_{\bar\beta_2} = \frac{b_{12}}{b_{11}} f_{\bar\beta_1} + c_{s,1} , \quad f_{\bar\beta_2} = \frac{b_{12}}{b_{11}} f_{\bar\beta_1} - c_{s,1} \tag{9.77}$$

hold maximum distance. Shifting f_1 within its interval $-f_{s,1}, \ldots, f_{s,1}$, the coordinates $(f_{\bar\beta_1}, f_{\bar\beta_2})$, as defined through (9.77), slide along two of the edges of the geometrical figure to be constructed. Obviously, the pertaining vertices follow from (9.72) and (9.75),

$$f_{\bar\beta_1} = b_{11} f_1 + b_{21} f_2^* + b_{31} f_3^* + b_{41} f_4^* + b_{51} f_5^* ,$$
$$f_{\bar\beta_2} = b_{12} f_1 + b_{22} f_2^* + b_{32} f_3^* + b_{42} f_4^* + b_{52} f_5^* . \tag{9.78}$$

We finally have found two of the polygon edges and the associated vertices.

Elimination of the other variables $f_2, f_3, \ldots, f_m$ ($m = 5$ here) reveals that there will be m pairs of parallel edges at most and, in particular, that the figure in question will be a convex polygon.

Should b_{11}, for example vanish, it would not be possible to eliminated f_1. Instead, (9.72) would yield two abscissas

$$f_{\bar\beta_1} = \pm [\, \operatorname{sign}(b_{21})\, b_{21} f_{s,2} + \operatorname{sign}(b_{31})\, b_{31} f_{s,3}$$
$$+ \operatorname{sign}(b_{41})\, b_{41} f_{s,4} + \operatorname{sign}(b_{51})\, b_{51} f_{s,5} \,] , \tag{9.79}$$

through each of which we may draw a vertical line parallel to the $f_{\bar\beta_2}$-axis. Along these vertical lines the coordinate $f_{\bar\beta_2}$ slides according to

$$f_{\bar\beta_2} = b_{12} f_1 \pm [\, \operatorname{sign}(b_{21})\, b_{22} f_{s,2} + \operatorname{sign}(b_{31})\, b_{32} f_{s,3}$$
$$+ \operatorname{sign}(b_{41})\, b_{42} f_{s,4} + \operatorname{sign}(b_{51})\, b_{52} f_{s,5} \,] . \tag{9.80}$$

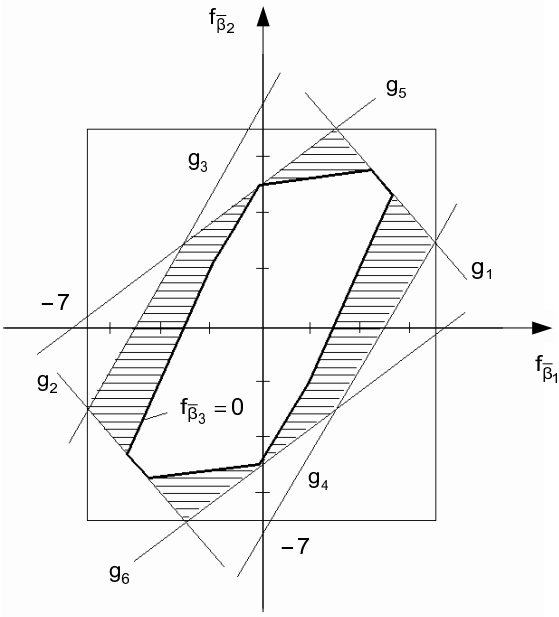


Fig. 9.3. Convex, point-symmetric polygon, $m = 4$

Example

We shall find the polygon defined by

$$\boldsymbol{B}^{\mathrm{T}} = \begin{bmatrix} 1 & 2 & 3 & -1 \\ -1 & 3 & 2 & 1 \end{bmatrix} \quad \text{and} \quad -1 \le f_i \le 1\,; \quad i = 1, \ldots, 4\,.$$

From

$$f_{\bar{\beta}_1} = f_1 + 2f_2 + 3f_3 - f_4\,; \quad f_{\bar{\beta}_2} = -f_1 + 3f_2 + 2f_3 + f_4$$

we conclude that the polygon is bounded by a rectangle of size

$$-7 \le f_{\bar{\beta}_1} \le 7\,; \quad -7 \le f_{\bar{\beta}_2} \le 7\,.$$

Furthermore, we see that there are, instead of four, just three pairs of straight lines, namely

$$\begin{aligned} (g_1, g_2): &\quad f_{\bar{\beta}_2} = -f_{\bar{\beta}_1} \pm 10\,, \\ (g_3, g_4): &\quad f_{\bar{\beta}_2} = \frac{3}{2} f_{\bar{\beta}_1} \pm \frac{15}{2}\,, \\ (g_5, g_6): &\quad f_{\bar{\beta}_2} = \frac{2}{3} f_{\bar{\beta}_1} \pm 5\,. \end{aligned}$$

Figure 9.3 depicts the polygon.

Remark: In least squares, treating r unknowns, we may happen to be interested in the couplings between $r' < r$ estimators wanting to assign to the remaining $r - r'$ any fixed values. Considering such a situation, we add to the relations for $f_{\bar{\beta}_1}$ and $f_{\bar{\beta}_2}$ some third relation for $f_{\bar{\beta}_3}$. Let the new system be given by

$$\begin{aligned} f_{\bar{\beta}_1} &= f_1 + 2f_2 + 3f_3 - f_4 \\ f_{\bar{\beta}_2} &= -f_1 + 3f_2 + 2f_3 + f_4 \\ f_{\bar{\beta}_3} &= 2f_1 - f_2 + 3f_3 + 3f_4\,, \end{aligned}$$

and let us look for the contour line $f_{\bar{\beta}_3} = 0$. Obviously, we have to consider the so-enlarged system as a whole, which, of course, leads us to a result quite different from that we got by treating the first two relations alone. Indeed, as Fig. 9.3 illustrates, the inner polygon depicting the new result encloses a smaller area than the previous outer one.

Security Polyhedra

We shall now investigate the geometrical properties of the solids established by three propagated systematic errors. Exemplifying the case $m = 5$, we consider

$$\begin{aligned} f_{\bar{\beta}_1} &= b_{11}f_1 + b_{21}f_2 + b_{31}f_3 + b_{41}f_4 + b_{51}f_5 \\ f_{\bar{\beta}_2} &= b_{12}f_1 + b_{22}f_2 + b_{32}f_3 + b_{42}f_4 + b_{52}f_5 \\ f_{\bar{\beta}_3} &= b_{13}f_1 + b_{23}f_2 + b_{33}f_3 + b_{43}f_4 + b_{53}f_5\,, \end{aligned} \tag{9.81}$$

where

$$-f_{s,i} \le f_i \le f_{s,i}\,; \quad i = 1, \ldots, 5 \tag{9.82}$$

is assumed. With respect to a rectangular $f_{\bar{\beta}_1}, f_{\bar{\beta}_2}, f_{\bar{\beta}_3}$ coordinate system, the solid in question is enclosed within a cuboid as given by (9.71). Writing (9.81) in the form

$$\begin{aligned} b_{11}f_1 + b_{21}f_2 + b_{31}f_3 &= f_{\bar{\beta}_1} - b_{41}f_4 - b_{51}f_5 = \xi \\ b_{12}f_1 + b_{22}f_2 + b_{32}f_3 &= f_{\bar{\beta}_2} - b_{42}f_4 - b_{52}f_5 = \eta \\ b_{13}f_1 + b_{23}f_2 + b_{33}f_3 &= f_{\bar{\beta}_3} - b_{43}f_4 - b_{53}f_5 = \zeta \end{aligned} \tag{9.83}$$

we may solve for f_3,

$$f_3 \begin{vmatrix} b_{11} & b_{21} & b_{31} \\ b_{12} & b_{22} & b_{32} \\ b_{13} & b_{23} & b_{33} \end{vmatrix} = \begin{vmatrix} b_{11} & b_{21} & \xi \\ b_{12} & b_{22} & \eta \\ b_{13} & b_{23} & \zeta \end{vmatrix}\,.$$

Defining

$$\lambda_{12} = b_{12}b_{23} - b_{22}b_{13}\,, \quad \mu_{12} = b_{21}b_{13} - b_{11}b_{23}\,, \quad \nu_{12} = b_{11}b_{22} - b_{21}b_{12}$$

we have

$$\lambda_{12} f_{\bar{\beta}_1} + \mu_{12} f_{\bar{\beta}_2} + \nu_{12} f_{\bar{\beta}_3} = c_{12}\,, \tag{9.84}$$

where

$$c_{12} = h_{12,3} f_3 + h_{12,4} f_4 + h_{12,5} f_5 \tag{9.85}$$

and

$$\begin{aligned} h_{12,3} &= (\lambda_{12} b_{31} + \mu_{12} b_{32} + \nu_{12} b_{33}) \\ h_{12,4} &= (\lambda_{12} b_{41} + \mu_{12} b_{42} + \nu_{12} b_{43}) \\ h_{12,5} &= (\lambda_{12} b_{51} + \mu_{12} b_{52} + \nu_{12} b_{53})\,. \end{aligned}$$

Solving (9.83) for f_3, the variables f_1 and f_2 vanish. Varying c_{12}, which is possible through f_3, f_4, f_5, the plane (9.84) gets shifted parallel to itself. The choices

$$\begin{aligned} f_3 = f_3^* &= \operatorname{sign}(h_{12,3})\, f_{s,3} \\ f_4 = f_4^* &= \operatorname{sign}(h_{12,4})\, f_{s,4} \\ f_5 = f_5^* &= \operatorname{sign}(h_{12,5})\, f_{s,5} \end{aligned}$$

assign a maximum value to c_{12},

$$c_{s,12} = h_{12,3} f_3^* + h_{12,4} f_4^* + h_{12,5} f_5^*$$

so that

$$-c_{s,12} \le c_{12} \le c_{s,12}\,.$$

Finally, we have found two of the faces of the solid, namely

$$\begin{aligned} \lambda_{12} f_{\bar{\beta}_1} + \mu_{12} f_{\bar{\beta}_2} + \nu_{12} f_{\bar{\beta}_3} &= -c_{s,12} \quad \text{(F1)} \\ \lambda_{12} f_{\bar{\beta}_1} + \mu_{12} f_{\bar{\beta}_2} + \nu_{12} f_{\bar{\beta}_3} &= c_{s,12} \quad \text{(F2)}\,, \end{aligned} \tag{9.86}$$

where, for convenience, the faces have been designated by F1 and F2. Within the vector

$$\boldsymbol{f} = (f_1 \quad f_2 \quad f_3 \quad f_4 \quad f_5)^{\mathrm{T}}\,,$$

the variables f_1, f_2 are free, while the variables f_3, f_4, f_5 are fixed. If f_1, f_2 vary, the vector $\boldsymbol{f}_{\bar{\boldsymbol{\beta}}} = \boldsymbol{B}^{\mathrm{T}} \boldsymbol{f}$ slides along the faces (9.86). Cyclically swapping the variables, we successively find all the faces of the solid, which, as we now see, is a convex polyhedron. As Table 9.4 indicates, the maximum number of faces is given by $m(m-1)$. Table 9.5 visualizes the swapping procedure.

If in (9.81), e.g. b_{11} and b_{12} vanish, we cannot eliminate f_1. Moreover, as ν_{12} becomes zero, (9.86) represents a pair of planes parallel to the $f_{\bar{\beta}_3}$-axis,

$$\lambda_{12} f_{\bar{\beta}_1} + \mu_{12} f_{\bar{\beta}_2} = \pm c_{s,12}\,, \quad \nu_{12} = 0\,.$$

The cases $\lambda_{12} = 0$ and $\mu_{12} = 0$ may be treated correspondingly.

Table 9.4. Maximum number of faces of the polyhedron

×	$f_1 f_2$	$f_1 f_3$	$f_1 f_4$	$f_1 f_5$
×	×	$f_2 f_3$	$f_2 f_4$	$f_2 f_5$
×	×	×	$f_3 f_4$	$f_3 f_5$
×	×	×	×	$f_4 f_5$
×	×	×	×	×

Table 9.5. Cyclic elimination, $r = 3$ and $m = 5$

	eliminated variable			variables remaining within the system		
1st step	f_1	f_2	⇒	f_3	f_4	f_5
2nd step	f_1	f_3	⇒	f_4	f_5	f_2
3rd step	f_1	f_4	⇒	f_5	f_2	f_3
4th step	f_1	f_5	⇒	f_2	f_3	f_4
5th step	f_2	f_3	⇒	f_4	f_5	f_1
6th step	f_2	f_4	⇒	f_5	f_1	f_3
7th step	f_2	f_5	⇒	f_1	f_3	f_4
8th step	f_3	f_4	⇒	f_5	f_1	f_2
9th step	f_3	f_5	⇒	f_1	f_2	f_4
10th step	f_4	f_5	⇒	f_1	f_2	f_3

Vertices

The vertices on the faces (9.86) emerge as follows. Given $h_{12,i} \neq 0$; $i = 3, 4, 5$, we consider, as f_3, f_4 and f_5 are fixed, two sets of $\boldsymbol{f}$-vectors referring to F1 and F2, namely

$$\begin{bmatrix} -f_{s,1} & -f_{s,2} & -f_3^* & -f_4^* & -f_5^* \end{bmatrix}^{\mathrm{T}} \\ \begin{bmatrix} f_{s,1} & -f_{s,2} & -f_3^* & -f_4^* & -f_5^* \end{bmatrix}^{\mathrm{T}} \\ \begin{bmatrix} -f_{s,1} & f_{s,2} & -f_3^* & -f_4^* & -f_5^* \end{bmatrix}^{\mathrm{T}} \\ \begin{bmatrix} f_{s,1} & f_{s,2} & -f_3^* & -f_4^* & -f_5^* \end{bmatrix}^{\mathrm{T}} \qquad \text{(F1)}$$

and

$$\begin{bmatrix} f_{s,1} & f_{s,2} & f_3^* & f_4^* & f_5^* \end{bmatrix}^{\mathrm{T}} \\ \begin{bmatrix} -f_{s,1} & f_{s,2} & f_3^* & f_4^* & f_5^* \end{bmatrix}^{\mathrm{T}} \\ \begin{bmatrix} f_{s,1} & -f_{s,2} & f_3^* & f_4^* & f_5^* \end{bmatrix}^{\mathrm{T}} \\ \begin{bmatrix} -f_{s,1} & -f_{s,2} & f_3^* & f_4^* & f_5^* \end{bmatrix}^{\mathrm{T}} \qquad \text{(F2)}$$

On each of the planes, these vectors mark exactly four vertices via $\boldsymbol{f}_{\bar{\boldsymbol{\beta}}} = \boldsymbol{B}^{\mathrm{T}} \boldsymbol{f}$. If in (9.85), e.g. $h_{12,5}$ vanishes, we would encounter eight vertices instead of

four on each of the faces (9.86). Should $h_{12,4}$ also be zero, there would be 16 vertices on each face. However, at least one of the coefficients $h_{12,i}$, $i = 3, 4, 5$ must be unequal to zero as otherwise the plane (9.84) would pass through the origin.

Contour Lines

Let us assume that none of the coefficients of the variables $f_{\bar{\beta}_k}$; $k = 1, 2, 3$ in (9.84) vanishes. Solving (9.86) for $f_{\bar{\beta}_2}$ yields

$$\begin{aligned} f_{\bar{\beta}_2} &= -\frac{\lambda_{12}}{\mu_{12}} f_{\bar{\beta}_1} - \frac{c_{s,12}}{\mu_{12}} - \frac{\nu_{12}}{\mu_{12}} f_{\bar{\beta}_3} \qquad \text{(F1)} \\ f_{\bar{\beta}_2} &= -\frac{\lambda_{12}}{\mu_{12}} f_{\bar{\beta}_1} + \frac{c_{s,12}}{\mu_{12}} - \frac{\nu_{12}}{\mu_{12}} f_{\bar{\beta}_3}\,. \qquad \text{(F2)} \end{aligned} \tag{9.87}$$

Obviously, any fixed $f_{\bar{\beta}_3}$ according to

$$\begin{aligned} f_{\bar{\beta}_3} &= b_{13} f_1 + b_{23} f_2 - b_{33} f_3^* - b_{43} f_4^* - b_{53} f_5^* = \text{const.} \qquad \text{(F1)} \\ f_{\bar{\beta}_3} &= b_{13} f_1 + b_{23} f_2 + b_{33} f_3^* + b_{43} f_4^* + b_{53} f_5^* = \text{const.} \qquad \text{(F2)} \end{aligned} \tag{9.88}$$

yields an $f_{\bar{\beta}_1}, f_{\bar{\beta}_2}$ contour line along the pertaining face of the polyhedron. For F2 we have

$$\begin{aligned} f_{\bar{\beta}_{3,2}} &= |b_{13}|\, f_{s,1} + |b_{23}|\, f_{s,2} + b_{33} f_3^* + b_{43} f_4^* + b_{53} f_5^* \\ f_{\bar{\beta}_{3,1}} &= -|b_{13}|\, f_{s,1} - |b_{23}|\, f_{s,2} + b_{33} f_3^* + b_{43} f_4^* + b_{53} f_5^* \end{aligned}$$

so that the interval

$$f_{\bar{\beta}_{3,1}} \le f_{\bar{\beta}_3} \le f_{\bar{\beta}_{3,2}} \qquad \text{(F2)} \tag{9.89}$$

constitutes the range of admissible $f_{\bar{\beta}_3}$ values for contour lines alongside F2. Analogously, for F1 we find

$$-f_{\bar{\beta}_{3,2}} \le f_{\bar{\beta}_3} \le -f_{\bar{\beta}_{3,1}}\,. \qquad \text{(F1)} \tag{9.90}$$

We may repeat this procedure with each of the $m(m-1)/2$ available pairs of parallel planes of the kind (9.86). Then, choosing any contour level $f_{\bar{\beta}_3} = \text{const.}$ within the interval

$$-f_{s,\bar{\beta}_3}, \ldots, f_{s,\bar{\beta}_3}$$

as defined in (9.71), we combine all straight lines of the kind (9.87) which possess an $f_{\bar{\beta}_3}$-value coping with this preset level. The search for the set of straight lines which actually constitutes a specific contour line $f_{\bar{\beta}_3} = \text{const.}$ is based on intervals of the kind (9.89) and (9.90). We then find the coordinates of the endpoints of the segments of the straight lines and string the segments

together thus building a polygon, namely that which is defined by the intersection of a horizontal plane having height $f_{\bar{\beta}_3} = \text{const.}$ with the polyhedron. Stacking the contour lines on top of each other maps the polyhedron.

It might appear to be more advantageous to bring the polyhedron into being via its faces and not by its contour lines. On the other hand, we should bear in mind that the number of faces rises rapidly with m, thus provoking situations which might appear to be scarcely visually controllable. In the opinion of the author, it therefore seems to be simpler to refer to contour lines. As they appear stacked, the polyhedron's hull should be smoothed by means of a suitable image filter.[5]

Example

We shall find the surfaces and contour lines of the polyhedron

$$\boldsymbol{f}_{\bar{\beta}} = \boldsymbol{B}^{\mathrm{T}}\boldsymbol{f}\,; \quad \boldsymbol{B}^{\mathrm{T}} = \begin{pmatrix} 1 & 2 & 3 & -1 & 2 \\ -1 & 3 & 2 & 2 & -1 \\ 2 & -1 & -3 & 3 & -3 \end{pmatrix}\,; \quad -1 \le f_i \le 1\,; \quad i = 1, \ldots, 4\,.$$

As the linear system

$$\begin{aligned} f_{\bar{\beta}_1} &= f_1 + 2f_2 + 3f_3 - f_4 + 2f_5 \\ f_{\bar{\beta}_2} &= -f_1 + 3f_2 + 2f_3 + 2f_4 - f_5 \\ f_{\bar{\beta}_3} &= 2f_1 - f_2 - 3f_3 + 3f_4 - 3f_5 \end{aligned}$$

shows, the polyhedron is enclosed within the cuboid

$$-9 \le f_{\bar{\beta}_1} \le 9\,; \quad -9 \le f_{\bar{\beta}_2} \le 9\,; \quad -12 \le f_{\bar{\beta}_3} \le 12\,.$$

Cyclic elimination, Table 9.6 yields the coefficients λ, μ, ν and the constants $\pm c_s$ for (9.86) and (9.87). Figure 9.4 depicts the polyhedron.

Table 9.6. Cyclic elimination, $m = 5$, $r = 3$

	eliminated variable	λ	μ	ν	c_s	$f_{\bar{\beta}_{3,1}}$	$f_{\bar{\beta}_{3,2}}$
1	f_1, f_2	−5	−5	5	80	6	12
2	f_1, f_3	−1	−9	5	80	0	10
3	f_1, f_4	−7	5	1	76	2	12
4	f_1, f_5	5	−7	1	68	−6	4
5	f_2, f_3	−7	−3	−5	24	−6	2
6	f_2, f_4	11	5	7	38	−8	0
7	f_2, f_5	−10	−4	−8	38	−12	−4
8	f_3, f_4	12	6	8	42	−6	6
9	f_3, f_5	−9	−3	−7	34	−10	2
10	f_4, f_5	−3	−3	−3	24	−12	0

[5] I am grateful to my son Niels for designing and implementing the filter.

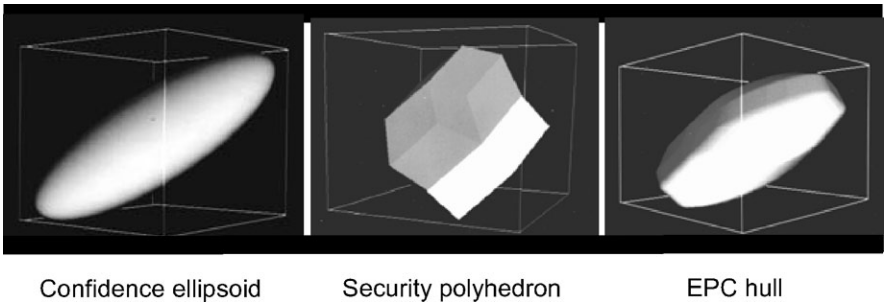


Fig. 9.4. Exemplary merging of a confidence ellipsoid and a security polyhedron into an **EPC** hull

Security Polytopes

Polyhedra in more than three dimensions, called polytopes, may be represented as a sequence of three-dimensional intersections each defining an $f_{\bar{\beta}_1}, f_{\bar{\beta}_2}, f_{\bar{\beta}_3}$ polyhedron. Let, for example, $r = 4$. It then would be possible to vary one of the propagated systematic errors, say $f_{\bar{\beta}_4}$, in discrete steps and display the associated sequence of polyhedra. Thus, the couplings would be mapped by an ensemble of polyhedra.

9.5.3 EP Boundaries and EPC Hulls

In the following, confidence ellipsoids and security polytopes will be merged into overall uncertainty spaces.

For $r = 2$ we have to combine confidence ellipses and security polygons, for $r = 3$ confidence ellipsoids and security polyhedra and for $r > 3$ abstract r-dimensional ellipsoids and polytopes.

The boundary of a two-dimensional overall uncertainty region turns out to be convex. As we shall see, the boundary consists of the arc segments of a contiguous decomposition of the circumference the **E**llipse and, additionally, of the edges of the **P**olygon, i.e. arcs and edges alternately succeed one another. We therefore will call these lines **EP** boundaries. In a sense, they resemble "convex slices of potatoes".

The boundary of a three-dimensional overall uncertainty space is also convex and comprises the segments of a contiguous decomposition of the **E**llipsoid's "skin", the faces of the **P**olyhedron and, finally, certain parts of elliptical **C**ylinders providing smooth transitions between flat and curved sections of the surface. So-established boundaries will be called **EPC** hulls. A comparison with "convex potatoes" appears suggestive.

EP Boundaries

We refer to (9.62),

$$\begin{aligned}\bar{\beta}_1 &= \beta_{0,1} + \left(\bar{\beta}_1 - \mu_{\bar{\beta}_1}\right) + f_{\bar{\beta}_1} \\ \bar{\beta}_2 &= \beta_{0,2} + \left(\bar{\beta}_2 - \mu_{\bar{\beta}_2}\right) + f_{\bar{\beta}_2}\,,\end{aligned} \tag{9.91}$$

and resort to Fig. 9.5 to tackle the task of designing a two-dimensional uncertainty region within which to find the true values $\beta_{0,1}, \beta_{0,2}$ of the estimators $\bar{\beta}_1, \bar{\beta}_2$. With respect to the influence of random errors, we refer to the confidence ellipsoid (9.66), as the parameters $\mu_{\bar{\beta}_1}, \mu_{\bar{\beta}_2}$ happen to be unknown. Because of

$$\boldsymbol{s}_{\bar{\boldsymbol{\beta}}}^{-1} = \left(\boldsymbol{B}^{\mathrm{T}}\boldsymbol{s}\,\boldsymbol{B}\right)^{-1} = \frac{1}{\left|\boldsymbol{s}_{\bar{\boldsymbol{\beta}}}\right|}\begin{pmatrix} s_{\bar{\beta}_2\bar{\beta}_2} & -s_{\bar{\beta}_1\bar{\beta}_2} \\ -s_{\bar{\beta}_2\bar{\beta}_1} & s_{\bar{\beta}_1\bar{\beta}_1}\end{pmatrix},$$

where $\left|\boldsymbol{s}_{\bar{\boldsymbol{\beta}}}\right| = s_{\bar{\beta}_1\bar{\beta}_1}s_{\bar{\beta}_2\bar{\beta}_2} - s^2_{\bar{\beta}_1\bar{\beta}_2}$, we arrive at

$$\begin{aligned}s_{\bar{\beta}_2\bar{\beta}_2}\left(\beta_1 - \bar{\beta}_1\right)^2 - 2s_{\bar{\beta}_1\bar{\beta}_2}\left(\beta_1 - \bar{\beta}_1\right)\left(\beta_2 - \bar{\beta}_2\right) + s_{\bar{\beta}_1\bar{\beta}_1}\left(\beta_1 - \bar{\beta}_2\right)^2 \\ = \left|\boldsymbol{s}_{\bar{\boldsymbol{\beta}}}\right|\frac{t^2_H(2,n)}{n}\,.\end{aligned} \tag{9.92}$$

To simplify the notation, we put

$$\begin{aligned}&x = \left(\beta_1 - \bar{\beta}_1\right)\,, \quad y = \left(\beta_2 - \bar{\beta}_2\right) \\ &a = s_{\bar{\beta}_2\bar{\beta}_2}\,, \quad b = -s_{\bar{\beta}_1\bar{\beta}_2}\,, \quad c = s_{\bar{\beta}_1\bar{\beta}_1}\,, \quad d = \left|\boldsymbol{s}_{\bar{\beta}}\right|\frac{t^2_H(2,n)}{n}\end{aligned}$$

so that

$$ax^2 + 2bxy + cy^2 = d\,. \tag{9.93}$$

Transforming the equation of the tangent to the ellipse (9.93) at the point $x = x_{\mathrm{E}}, y = y_{\mathrm{E}}$ into Hesse's normal form, we may easily find that point of the security polygon which maximizes the two-dimensional overall uncertainty region "outwardly". The slope of the tangent at $(x_{\mathrm{E}}, y_{\mathrm{E}})$,

$$y'_{\mathrm{E}} = -\frac{ax_{\mathrm{E}} + by_{\mathrm{E}}}{bx_{\mathrm{E}} + cy_{\mathrm{E}}} \tag{9.94}$$

leads to the equation

$$y = y_{\mathrm{E}} + y'_{\mathrm{E}}(x - x_{\mathrm{E}}) \tag{9.95}$$

of the tangent, the Hesse form of which is

$$-\frac{y'_{\mathrm{E}}}{H}x + \frac{1}{H}y + \frac{y'_{\mathrm{E}}x_{\mathrm{E}} - y_{\mathrm{E}}}{H} = 0\,, \tag{9.96}$$

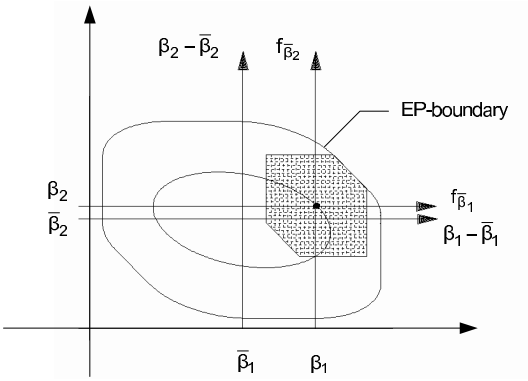


Fig. 9.5. EP boundary localizing the true values $\beta_{0,1}, \beta_{0,2}$

where

$$H = -\text{sign}\,(y'_{\text{E}} x_{\text{E}} - y_{\text{E}}) \sqrt{1 + {y'_E}^2}\,.$$

Let the $(\xi_{\text{P}}, \eta_{\text{P}})$; $P = 1, 2, \ldots$ denote the vertices of the polygon with respect to a rectangular, body-fixed $f_{\bar{\beta}_1}, f_{\bar{\beta}_2}$ coordinate system. For a given point $(x_{\text{E}}, y_{\text{E}})$, we successively insert the coordinates of the vertices $(\xi_{\text{P}}, \eta_{\text{P}})$; $P = 1, 2, \ldots$ in (9.96) and select that vertex which produces the largest positive distance according to

$$-\frac{y'_{\text{E}}}{H}\,(x_{\text{E}} + \xi_{\text{P}}) + \frac{1}{H}\,(y_{\text{E}} + \eta_{\text{P}}) + \frac{y'_{\text{E}} x_{\text{E}} - y_{\text{E}}}{H} > 0\,; \quad P = 1, 2, \ldots\,. \tag{9.97}$$

Obviously, the coordinates

$$x_{\text{EP}} = x_{\text{E}} + \xi_{\text{P}}\,; \quad y_{\text{EP}} = y_{\text{E}} + \eta_{\text{P}} \tag{9.98}$$

define a point of the boundary we are looking for. Now, all we have to do is to move $(x_{\text{E}}, y_{\text{E}})$ in discrete steps along the circumference of the ellipse and to restart procedure (9.97) thus bringing into being, bit by bit, the boundary of the two-dimensional uncertainty region sought after. According to the error model, this line localizes the true values $\beta_{0,1}, \beta_{0,2}$ "quasi-certainly".

If the tangent runs parallel to one of the edges of the polygon, that edge as a whole becomes part of the boundary. Consider two successive points $(x_{\text{E}}, y_{\text{E}}), (x_{\text{E}'}, y_{\text{E}'})$, the tangents of which are parallel to polygon edges. Then, the arc segment lying in-between becomes, as shifted "outwardly", part of the boundary. Hence, the circumference of the ellipse gets contiguously decomposed, and each of its segments becomes part of the boundary of the two-dimensional uncertainty region. Finally, this line is made up of **E**lliptical arcs and **P**olygon edges. From this the term **EP** boundary has been derived.

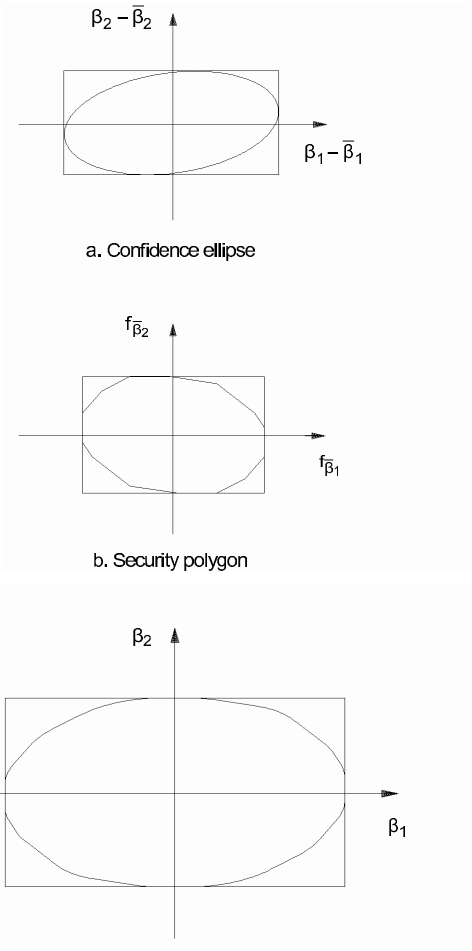


Fig. 9.6. Exemplary merging of a confidence interval and a security polygon

Example

We shall merge the confidence ellipse

$$\boldsymbol{s}_{\bar{\boldsymbol{\beta}}} = \begin{pmatrix} 500 & 70 \\ 70 & 200 \end{pmatrix} ; \quad t_P(2,n)/\sqrt{n} = 1$$

and the security polygon

$$\boldsymbol{B}^{\mathrm{T}} = \begin{pmatrix} 1 & 2 & 3 & -1 & 5 & -1 & 7 & 0 & -3 & 8 \\ -1 & 3 & 2 & 1 & -1 & 2 & 0 & 2 & 7 & -1 \end{pmatrix}$$

$$-1 \le f_i \le 1 ; \quad i = 1, \ldots, 10$$

into an overall uncertainty region or **EP** boundary.

According to Sect. 3.6, the confidence ellipse is bounded by a rectangle with sides

$$\sqrt{s_{\bar{\beta}_1\bar{\beta}_1}} = \sqrt{500} = \pm 22.4\,, \quad \sqrt{s_{\bar{\beta}_2\bar{\beta}_2}} = \sqrt{200} = \pm 14.1\,.$$

The rectangle which encloses the security polygon has dimensions

$$\pm 31 \quad \text{and} \quad \pm\, 20\,.$$

But then the **EP** boundary is contained in a rectangle with sides

$$\pm 53.4 \quad \text{and} \quad \pm\, 34.1\,.$$

Figure 9.6 illustrates the computer-aided putting together of the two figures.

EPC Hulls

Adding component $\bar{\beta}_3$ according to (9.62),

$$\begin{aligned} \bar{\beta}_1 &= \beta_{0,1} + \left(\bar{\beta}_1 - \mu_{\bar{\beta}_1}\right) + f_{\bar{\beta}_1} \\ \bar{\beta}_2 &= \beta_{0,2} + \left(\bar{\beta}_2 - \mu_{\bar{\beta}_2}\right) + f_{\bar{\beta}_2} \\ \bar{\beta}_3 &= \beta_{0,3} + \left(\bar{\beta}_3 - \mu_{\bar{\beta}_3}\right) + f_{\bar{\beta}_3} \end{aligned} \tag{9.99}$$

we may proceed as for two-dimensional uncertainty regions. Let us consider the simplest case: We place the center of the security polyhedron at some point $(x_\mathrm{E}, y_\mathrm{E}, z_\mathrm{E})$ of the ellipsoid's "skin" and shift the tangent plane at this point outwardly until it passes through that vertex of the polyhedron which maximizes the uncertainty space in question. The associate vertex $(\xi_\mathrm{P}, \eta_\mathrm{P}, \zeta_\mathrm{P})$ is found by trial and error. Finally, the coordinates

$$\begin{aligned} x_\mathrm{EPZ} &= x_\mathrm{E} + \xi_\mathrm{P} \\ y_\mathrm{EPZ} &= y_\mathrm{E} + \mu_\mathrm{P} \\ z_\mathrm{EPZ} &= z_\mathrm{E} + \zeta_\mathrm{P} \end{aligned} \tag{9.100}$$

provide a point of the **EPC** hull to be constructed.

To begin with, we shall find a suitable representation of the tangent plane to the confidence ellipsoid. For convenience, we denote the inverse of the empirical variance–covariance matrix entering (9.66) merely symbolically, i.e. in

$$\frac{t_P^2\,(3,n)}{n} = \left(\boldsymbol{\beta} - \bar{\boldsymbol{\beta}}\right)^\mathrm{T} \left(\boldsymbol{B}^\mathrm{T}\boldsymbol{s}\,\boldsymbol{B}\right)^{-1} \left(\boldsymbol{\beta} - \bar{\boldsymbol{\beta}}\right)$$

we set

$$\left(\boldsymbol{B}^\mathrm{T}\boldsymbol{s}\,\boldsymbol{B}\right)^{-1} = \begin{pmatrix} \gamma_{11} & \gamma_{12} & \gamma_{13} \\ \gamma_{21} & \gamma_{22} & \gamma_{23} \\ \gamma_{31} & \gamma_{32} & \gamma_{33} \end{pmatrix}\,.$$

Defining

$$x = \left(\beta_1 - \bar{\beta}_1\right) , \quad y = \left(\beta_2 - \bar{\beta}_2\right) , \quad z = \left(\beta_3 - \bar{\beta}_3\right) , \quad d = t_P^2 \left(3, n\right) / n ,$$

the confidence ellipsoid turns into

$$\gamma_{11} x^2 + \gamma_{22} y^2 + \gamma_{33} z^2 + 2\gamma_{12} xy + 2\gamma_{23} yz + 2\gamma_{31} zx = d . \tag{9.101}$$

We now intersect the ellipsoid by a set of sufficiently close-spaced planes $z_{\mathrm{E}} = \text{const.}$, where

$$-\frac{t_P^2 \left(r, n\right)}{n} \sqrt{s_{\bar{\beta}_3 \bar{\beta}_3}} \leq z_{\mathrm{E}} \leq \frac{t_P^2 \left(r, n\right)}{n} \sqrt{s_{\bar{\beta}_3 \bar{\beta}_3}} , \tag{9.102}$$

and shift the center of the polyhedron in discrete steps alongside any particular contour line $z_{\mathrm{E}} = \text{const.}$ of the ellipsoid's "skin". During this slide, the spatial orientation of the polyhedron remains fixed. At each stop $(x_{\mathrm{E}}, y_{\mathrm{E}}, z_{\mathrm{E}})$ we construct the tangent plane

$$n_x \left(x - x_{\mathrm{E}}\right) + n_y \left(y - y_{\mathrm{E}}\right) + n_z \left(z - z_{\mathrm{E}}\right) = 0 , \tag{9.103}$$

where the n_x, n_y, n_y denote the components of the normal

$$\boldsymbol{n} = \begin{pmatrix} n_x \\ n_y \\ n_y \end{pmatrix} = \begin{pmatrix} \gamma_{11} x_{\mathrm{E}} + \gamma_{12} y_{\mathrm{E}} + \gamma_{31} z_{\mathrm{E}} \\ \gamma_{12} x_{\mathrm{E}} + \gamma_{22} y_{\mathrm{E}} + \gamma_{23} z_{\mathrm{E}} \\ \gamma_{31} x_{\mathrm{E}} + \gamma_{23} y_{\mathrm{E}} + \gamma_{33} z_{\mathrm{E}} \end{pmatrix} \tag{9.104}$$

at $(x_{\mathrm{E}}, y_{\mathrm{E}}, z_{\mathrm{E}})$. By means of Hesse's normal form

$$\frac{n_x}{H} x + \frac{n_y}{H} y + \frac{n_z}{H} z - \frac{\left(n_x x_{\mathrm{E}} + n_y y_{\mathrm{E}} + n_z z_{\mathrm{E}}\right)}{H} = 0 , \tag{9.105}$$

where

$$H = \mathrm{sign} \left(n_x x_{\mathrm{E}} + n_y y_{\mathrm{E}} + n_z z_{\mathrm{E}}\right) \sqrt{n_x^2 + n_y^2 + n_z^2} ,$$

we are in a position to select that vertex of the polyhedron which maximizes the size of the three-dimensional uncertainty region "outwardly". This is easily done by successively inserting the vertices $(\xi_{\mathrm{P}}, \eta_{\mathrm{P}}, \zeta_{\mathrm{P}})$; $P = 1, 2, \ldots$ of the polyhedron into (9.105), i.e. by testing the expressions

$$\begin{aligned} &\frac{n_x}{H} \left(x_{\mathrm{E}} + \xi_{\mathrm{P}}\right) + \frac{n_y}{H} \left(y_{\mathrm{E}} + \eta_{\mathrm{P}}\right) + \frac{n_z}{H} \left(z_{\mathrm{E}} + \zeta_{\mathrm{P}}\right) \\ &- \frac{\left(n_x x_{\mathrm{E}} + n_y y_{\mathrm{E}} + n_z z_{\mathrm{E}}\right)}{H} > 0 . \quad P = 1, 2, \ldots \end{aligned} \tag{9.106}$$

one after another. It goes without saying that the points $(x_{\mathrm{E}}, y_{\mathrm{E}}, z_{\mathrm{E}} = \text{const.})$ of a given contour line of the ellipsoid will not produce a contour line of

the three-dimensional uncertainty region in question. After all, this region is established through a dense system of curved, non-intersecting lines (9.100). To improve the graphical appearance of the stripy surface pattern we resort to a smoothing filtering algorithm[6] and a suitable "illumination" procedure.

As can be shown, the construction procedure implies a contiguous decomposition of the **E**llipsoid's "skin". These segments, shifted "outwardly", become integral parts of the hull. The same applies to each of the faces of the **P**olyhedron. Finally, polyhedron edges when shifted appropriately alongside the ellipsoid's skin, produce segments of elliptically curved **C**ylinders.

The itemized geometrical constituents, adjoining smoothly, have led to the term **EPC** hull.

Example

We shall merge the confidence ellipsoid

$$\boldsymbol{s}_{\bar{\beta}} = \begin{pmatrix} 121 & -70 & -80 \\ -70 & 100 & 50 \\ -80 & 50 & 81 \end{pmatrix} ; \qquad t_P(3,n)/\sqrt{n} = 1$$

and the security polyhedron

$$\boldsymbol{B}^{\mathrm{T}} = \begin{pmatrix} 1 & 2 & 3 & -1 & 2 \\ -1 & 3 & 2 & 2 & -1 \\ 2 & -1 & -3 & 3 & -3 \end{pmatrix} ; \quad -1 \le f_i \le 1$$

into an **EPC** hull.

The ellipsoid, polyhedron and **EPC** hull are enclosed within cuboids the side lengths of which are given by

$$\pm 11, \pm 10, \pm 9\,; \quad \pm 9, \pm 9, \pm 12 \quad \text{and} \quad \pm\, 20, \pm 19, \pm 21\,,$$

respectively.

[6] I am grateful to my son Niels for designing and implementing the filter.

Part III

Special Linear and Linearized Systems

10 Systems with Two Parameters

10.1 Straight Lines

On fitting of a straight line through m given data pairs we refer to three metrologically different situations. In the simplest case, we assume, by definition, the abscissas to be error-free and the ordinates to be individual, erroneous measurements

$$(x_{0,1}, y_1)\ , \quad (x_{0,2}, y_2), \ldots, (x_{0,m}, y_m)\ . \tag{10.1}$$

Next, again considering error-free abscissas, we assume the ordinates to be arithmetic means

$$(x_{0,1}, \bar{y}_1)\ , \quad (x_{0,2}, \bar{y}_2), \ldots, (x_{0,m}, \bar{y}_m)\ . \tag{10.2}$$

In general, however, both coordinates will exhibit the structure of arithmetic means

$$(\bar{x}_1, \bar{y}_1)\ , \quad (\bar{x}_2, \bar{y}_2), \ldots, (\bar{x}_m, \bar{y}_m)\ . \tag{10.3}$$

Let the latter be based on n repeat measurements x_{il}, y_{il}, $l = 1, \ldots, n$,

$$\bar{x}_i = \frac{1}{n}\sum_{l=1}^{n} x_{il} = x_{0,i} + (\bar{x}_i - \mu_{\bar{x}_i}) + f_{\bar{x}_i}\,; \quad f_{s,\bar{x}_i} \le f_{\bar{x}_i} \le f_{s,\bar{x}_i}$$

$$\bar{y}_i = \frac{1}{n}\sum_{l=1}^{n} y_{il} = y_{0,i} + (\bar{y}_i - \mu_{\bar{y}_i}) + f_{\bar{y}_i}\,; \quad f_{s,\bar{y}_i} \le f_{\bar{y}_i} \le f_{s,\bar{y}_i}\,.$$

The data pairs (10.2) imply error bars

$$\bar{y}_i \pm u_{\bar{y}_i}\,; \quad i = 1, \ldots, m\,,$$

and the pairs (10.3) error rectangles

$$\bar{x}_i \pm u_{\bar{x}_i}\ , \quad \bar{y}_i \pm u_{\bar{y}_i}\,; \quad i = 1, \ldots, m\,.$$

Obviously, the data given in (10.1) should also exhibit error bars. However, the experimenter is not in a position to quote them when finishing his measurements. But, as will be shown, error bars turn out to be assessable afterwards, namely when a straight line has been fitted through the measured data.

Given that the measurements are based on a linear physical model, the true values $(x_{0,i},\, y_{0,i})$; $i = 1, \ldots, m$ of the coordinate pairs should establish a true straight line

$$y_0(x) = \beta_{0,1} + \beta_{0,2} x\,, \tag{10.4}$$

where $\beta_{0,1}$ and $\beta_{0,2}$ denote the true y intercept and the true slope. A necessary condition for this to occur comes from the error bars (and error rectangles). If the latter prove to be reliable, they will localize the true values $(x_{0,i},\, y_{0,i})$; $i = 1, \ldots, m$. Consequently, it should be possible to draw a straight line either through all error bars (and error rectangles) or, at least, through as many as possible. Error bars (or rectangles) lying too far apart so that they cannot be "hit" by the straight line do not fit the intersected ones. In the following we shall assume the linear model to be valid and, in the first step, assess the parameters

$$\bar{\beta}_k \pm u_{\bar{\beta}_k}\,; \quad k = 1, 2 \tag{10.5}$$

of the fitted straight line

$$\bar{y}(x) = \bar{\beta}_1 + \bar{\beta}_2 x\,. \tag{10.6}$$

In the second step we shall find a so-called uncertainty band

$$\bar{y}\,(x) \pm u_{\bar{y}(x)} \tag{10.7}$$

which we demand to enclose the true straight line (10.4).

Let us formalize a least squares adjustment based on the data pairs (10.3). The erroneous data give rise to the linear system

$$\bar{y}_i \approx \beta_1 + \beta_2\, \bar{x}_i\,; \quad i = 1, \ldots, m\,. \tag{10.8}$$

Introducing the vectors

$$\bar{\boldsymbol{y}} = (\bar{y}_1 \quad \bar{y}_2 \quad \cdots \quad \bar{y}_m)^{\mathrm{T}}\,, \quad \boldsymbol{\beta} = (\beta_1 \quad \beta_2)^{\mathrm{T}} \tag{10.9}$$

and the design matrix

$$\boldsymbol{A} = \begin{pmatrix} 1 & \bar{x}_1 \\ 1 & \bar{x}_2 \\ \cdots & \cdots \\ 1 & \bar{x}_m \end{pmatrix}\,, \tag{10.10}$$

(10.8) becomes

$$\boldsymbol{A}\boldsymbol{\beta} \approx \bar{\boldsymbol{y}}\,. \tag{10.11}$$

Obviously, the design matrix $\boldsymbol{A}$ includes erroneous quantities. Though this aspect remains irrelevant with respect to the orthogonal projection of the

vector $\bar{\boldsymbol{y}}$ onto the column space of the matrix $\boldsymbol{A}$, it will complicate the estimation of measurement uncertainties. The orthogonal projection through $\boldsymbol{P} = \boldsymbol{A}(\boldsymbol{A}^{\mathrm{T}}\boldsymbol{A})^{-1}\boldsymbol{A}^{\mathrm{T}}$ as defined in (7.13) turns (10.11) into

$$\boldsymbol{A}\bar{\boldsymbol{\beta}} = \boldsymbol{P}\bar{\boldsymbol{y}} \tag{10.12}$$

so that

$$\bar{\boldsymbol{\beta}} = \boldsymbol{B}^{\mathrm{T}}\bar{\boldsymbol{y}}\,; \quad \boldsymbol{B} = \boldsymbol{A}\left(\boldsymbol{A}^{\mathrm{T}}\boldsymbol{A}\right)^{-1}\,. \tag{10.13}$$

Denoting

$$\boldsymbol{B} = (b_{ik})\;; \quad i = 1, \ldots, m\,,\; k = 1, 2$$

the components $\bar{\beta}_1$, $\bar{\beta}_2$ of the solution vector $\bar{\boldsymbol{\beta}}$ take the form

$$\bar{\beta}_1 = \sum_{i=1}^{m} b_{i1}\bar{y}_i\,, \quad \bar{\beta}_2 = \sum_{i=1}^{m} b_{i2}\bar{y}_i\,. \tag{10.14}$$

Finally, the least squares adjustment has confronted the true straight line (10.4) with the approximation formally introduced in (10.6). Let us present the quantities b_{ik} detail. The inversion of the matrix

$$\boldsymbol{A}^{\mathrm{T}}\boldsymbol{A} = \begin{pmatrix} m & \sum\limits_{j=1}^{m} \bar{x}_j \\ \sum\limits_{j=1}^{m} \bar{x}_j & \sum\limits_{j=1}^{m} \bar{x}_j^2 \end{pmatrix} \tag{10.15}$$

yields

$$\left(\boldsymbol{A}^{\mathrm{T}}\boldsymbol{A}\right)^{-1} = \frac{1}{D}\begin{pmatrix} \sum\limits_{j=1}^{m} \bar{x}_j^2 & -\sum\limits_{j=1}^{m} \bar{x}_j \\ -\sum\limits_{j=1}^{m} \bar{x}_j & m \end{pmatrix}\;; \quad D = m\sum_{j=1}^{m} \bar{x}_j^2 - \left[\sum_{j=1}^{m} \bar{x}_j\right]^2 \tag{10.16}$$

so that

$$\boldsymbol{B} = \frac{1}{D}\begin{bmatrix} \sum\limits_{j=1}^{m} \bar{x}_j^2 - \bar{x}_1 \sum\limits_{j=1}^{m} \bar{x}_j & -\sum\limits_{j=1}^{m} \bar{x}_j + m\bar{x}_1 \\ \sum\limits_{j=1}^{m} \bar{x}_j^2 - \bar{x}_2 \sum\limits_{j=1}^{m} \bar{x}_j & -\sum\limits_{j=1}^{m} \bar{x}_j + m\bar{x}_2 \\ \cdots & \cdots \\ \sum\limits_{j=1}^{m} \bar{x}_j^2 - \bar{x}_m \sum\limits_{j=1}^{m} \bar{x}_j & -\sum\limits_{j=1}^{m} \bar{x}_j + m\bar{x}_m \end{bmatrix}, \tag{10.17}$$

and, letting $i = 1, \ldots, m$,

$$b_{i1} = \frac{1}{D}\left[\sum_{j=1}^{m} \bar{x}_j^2 - \bar{x}_i \sum_{j=1}^{m} \bar{x}_j\right] \; ; \quad b_{i2} = \frac{1}{D}\left[-\sum_{j=1}^{m} \bar{x}_j + m\bar{x}_i\right] \; . \tag{10.18}$$

In the special case of error-free abscissas, we merely need to substitute the true values $x_{0,j}$ for the means $\bar{x}_j$,

$$b_{i1} = \frac{1}{D}\left[\sum_{j=1}^{m} x_{0,j}^2 - x_{0,i} \sum_{j=1}^{m} x_{0,j}\right] \; ; \quad b_{i2} = \frac{1}{D}\left[-\sum_{j=1}^{m} x_{0,j} + m x_{0,i}\right] \tag{10.19}$$

where

$$D = m \sum_{j=1}^{m} x_{0,j}^2 - \left[\sum_{j=1}^{m} x_{0,j}\right]^2 \; .$$

10.1.1 Error-free Abscissas, Erroneous Ordinates

Though in most cases both the abscissas and the ordinates will be affected by measurement errors, the standard literature confines itself to the case of error-free abscissas. To begin with, we will follow this tradition, the subsequent section will, however, deal with the more general situation.

No Repeat Measurements

In the simplest case there is just one measured ordinate for each abscissa. Let us further assume that to each of the ordinates we may attribute one and the same systematic error, otherwise, under the present conditions, we would not be in a position to estimate uncertainties, see Sect. 8.2.

Summarizing, our premises are as follows: We assume

- the true values $(x_{0,i}, y_{0,i})$; $i = 1, \ldots, m$ to satisfy the linear model (10.4),
- the abscissas to be error-free,
- the random errors, superposed on the true values of the ordinates to be independent and to stem from one and the same parent distribution,
- each ordinate to carry one and the same systematic error $f_{y_i} = f_y$; $i = 1, \ldots, m$.

The input data

$$\begin{aligned} &\boldsymbol{y} = (y_1\, y_2\, \ldots\, y_m)^{\mathrm{T}} \\ &y_i = y_{0,i} + \varepsilon_i + f_y = y_{0,i} + (y_i - \mu_{y_i}) + f_y \, ; \quad -f_{s,y} \le f_y \le f_{s,y} \end{aligned} \tag{10.20}$$

and the design matrix

$$\boldsymbol{A} = \begin{pmatrix} 1 & x_{0,1} \\ 1 & x_{0,2} \\ \dots & \dots \\ 1 & x_{0,m} \end{pmatrix} \tag{10.21}$$

define the inconsistent system

$$\boldsymbol{A}\boldsymbol{\beta} \approx \boldsymbol{y} \tag{10.22}$$

to be submitted to least squares. The coefficients b_{i1} and b_{i2} of the estimators

$$\bar{\beta}_1 = \sum_{i=1}^{m} b_{i1} y_i \quad \text{and} \quad \bar{\beta}_2 = \sum_{i=1}^{m} b_{i\,2} y_i \tag{10.23}$$

have been quoted in (10.19). For convenience, let us collect the quantities defining the true linear system

$$\boldsymbol{A}\boldsymbol{\beta}_0 = \boldsymbol{y}_0\,, \quad \boldsymbol{\beta}_0 = (\beta_{0,1} \quad \beta_{0,2})^{\mathrm{T}}\,, \quad \boldsymbol{y}_0 = (y_{0,1}\, y_{0,2}\, \dots\, y_{0,m})^{\mathrm{T}}\,. \tag{10.24}$$

Here, $\boldsymbol{\beta}_0$ designates the true solution vector and $\boldsymbol{y}_0$ the vector of the true values of the observations.

Next we prove, given the above quoted conditions apply, the term $\boldsymbol{f}^{\mathrm{T}}\boldsymbol{f} - \boldsymbol{f}^{\mathrm{T}}\boldsymbol{P}\boldsymbol{f}$ appearing in (8.17) vanishes. To this end we refer to an auxiliary vector $\boldsymbol{\gamma}_0$. As on each of the ordinates one and the same systematic error f_y is superimposed, on account of

$$\boldsymbol{A}\boldsymbol{\gamma}_0 = \boldsymbol{y}_0 + \boldsymbol{f}\,; \quad \boldsymbol{f} = f_y\,(1\,1\,\dots\,1)^{\mathrm{T}} \tag{10.25}$$

$\boldsymbol{\gamma}_0$ has the components

$$\boldsymbol{\gamma}_0 = \begin{pmatrix} \gamma_{0,1} \\ \gamma_{0,2} \end{pmatrix} = \begin{pmatrix} \beta_{0,1} + f_y \\ \beta_{0,2} \end{pmatrix} \tag{10.26}$$

as, evidently, the slope $\beta_{0,2}$ is not subject to change. Combining (10.24) and (10.25) yields

$$\boldsymbol{A}\boldsymbol{\gamma}_0 = \boldsymbol{A}\boldsymbol{\beta}_0 + \boldsymbol{A}\begin{pmatrix} f_y \\ 0 \end{pmatrix} = \boldsymbol{A}\boldsymbol{\beta}_0 + \boldsymbol{f}\,,$$

i.e.

$$\boldsymbol{A}\begin{pmatrix} f_y \\ 0 \end{pmatrix} = \boldsymbol{f}\,, \quad \boldsymbol{P}\boldsymbol{f} = \boldsymbol{f} \Rightarrow \boldsymbol{f}^{\mathrm{T}}\boldsymbol{f} - \boldsymbol{f}^{\mathrm{T}}\boldsymbol{P}\boldsymbol{f} = \boldsymbol{0} \tag{10.27}$$

with $\boldsymbol{P} = \boldsymbol{A}(\boldsymbol{A}^{\mathrm{T}}\boldsymbol{A})^{-1}\boldsymbol{A}^{\mathrm{T}}$. Consequently, we may refer to (8.11) and estimate the unknown theoretical variance

$$\sigma^2 = E\left\{(Y_i - \mu_{y_i})^2\right\}\,; \quad \mu_{y_i} = E\{Y_i\}\,; \quad i = 1, \ldots, m$$

of the input data[1] through

$$s^2 = \frac{\bar{Q}_{\text{unweighted}}}{m-2} \tag{10.28}$$

so that, as shown in Sect. 8.2,

$$\frac{(m-2)\,s^2}{\sigma^2} = \frac{\bar{Q}_{\text{unweighted}}}{\sigma^2} = \chi^2\,(m-2)\,. \tag{10.29}$$

Finally, we are in a position to assign uncertainties to the individual measurements y_i, $i = 1, \ldots, m$. Referring to (3.49), Student's

$$T = \frac{(Y_i - \mu_{y_i})/\sigma}{S/\sigma} = \frac{(Y_i - \mu_{y_i})/\sigma}{\sqrt{[\chi^2(m-2)]\,/(m-2)}}\,; \quad i = 1, \ldots, m$$

enables us to define the confidence intervals

$$y_i - t_P(m-2)s \le \mu_{y_i} \le y_i + t_P(m-2)s\,; \quad i = 1, \ldots, m$$

for the expectations $\mu_{y_i} = E\{Y_i\}$. We then associate overall uncertainties of the kind

$$y_i \pm u_{y_i}\,; \quad u_{y_i} = t_P(m-2)s + f_{s,y}\,; \quad i = 1, \ldots, m \tag{10.30}$$

with the individual measurements y_i; $i = 1, \ldots, m$.

Uncertainties of the Components of the Solution Vector

Though, at present, there are no repeat measurements, we shall still denote estimators by a bar on top. Inserting (10.20) into (10.14) yields

$$\begin{aligned}\bar{\beta}_k &= \sum_{i=1}^{m} b_{ik}\,[y_{0,i} + (y_i - \mu_{y_i}) + f_y] \\ &= \beta_{0,k} + \sum_{i=1}^{m} b_{ik}\,(y_i - \mu_{y_i}) + f_y \sum_{i=1}^{m} b_{ik}\,; \quad k = 1, 2\,.\end{aligned} \tag{10.31}$$

The respective sums of the coefficients b_{i1} and b_{i2}, as defined in (10.19), are given by

[1] If, in contrast to our premise, the systematic errors vary along the sequence of measured ordinates, or should the fitted line deviate too much at its left and right "ends" from the empirical data pairs implying that the latter do not fulfil the linear model (10.4), the estimator (10.28) will, of course, break down.

$$\sum_{i=1}^{m} b_{i1} = 1 \quad \text{and} \quad \sum_{i=1}^{m} b_{i2} = 0 \tag{10.32}$$

so that the third term on the right-hand side of (10.31) gives the propagated systematic errors

$$f_{\bar{\beta}_1} = f_y \quad \text{and} \quad f_{\bar{\beta}_2} = 0\,. \tag{10.33}$$

The empirical variance–covariance matrix of the solution vector

$$\boldsymbol{s}_{\bar{\beta}} = \begin{pmatrix} s_{\bar{\beta}_1\bar{\beta}_1} & s_{\bar{\beta}_1\bar{\beta}_2} \\ s_{\bar{\beta}_2\bar{\beta}_1} & s_{\bar{\beta}_2\bar{\beta}_2} \end{pmatrix} \tag{10.34}$$

can only be stated in analogy to the way the conventional error calculus proceeds, i.e. we firstly define a theoretical variance–covariance matrix and subsequently substitute empirical quantities for the inaccessible theoretical quantities. Denoting the expectations of the components $\bar{\beta}_1, \bar{\beta}_2$ of the solution vector as

$$\mu_{\bar{\beta}_1} = \sum_{i=1}^{m} b_{i1}\mu_{y_i}\,, \quad \mu_{\bar{\beta}_2} = \sum_{i=1}^{m} b_{i2}\mu_{y_i}\,; \quad \mu_{y_i} = E\{Y_i\} \tag{10.35}$$

the theoretical variances and the theoretical covariance turn out to be

$$\begin{aligned} \sigma^2_{\bar{\beta}_1} \equiv \sigma_{\bar{\beta}_1\bar{\beta}_1} &= E\left\{\left(\bar{\beta}_1 - \mu_{\bar{\beta}_1}\right)^2\right\} \\ &= E\left\{\left[\sum_{i=1}^{m} b_{i1}\left(Y_i - \mu_{y_i}\right)\right]^2\right\} = \sigma^2 \sum_{i=1}^{m} b_{i1}^2 \\ \sigma^2_{\bar{\beta}_2} \equiv \sigma_{\bar{\beta}_2\bar{\beta}_2} &= \sigma^2 \sum_{i=1}^{m} b_{i2}^2 \end{aligned} \tag{10.36}$$

and

$$\sigma_{\bar{\beta}_1\bar{\beta}_2} = \sigma^2 \sum_{i=1}^{m} b_{i1} b_{i2} \tag{10.37}$$

respectively. Obviously, their empirical counterparts are

$$\begin{aligned} s_{\bar{\beta}_1\bar{\beta}_1} = s^2_{\bar{\beta}_1} = s^2 \sum_{i=1}^{m} b_{i1}^2\,, \quad s_{\bar{\beta}_2\bar{\beta}_2} = s^2_{\bar{\beta}_2} = s^2 \sum_{i=1}^{m} b_{i2}^2\,, \\ s_{\bar{\beta}_1\bar{\beta}_2} = s^2 \sum_{i=1}^{m} b_{i1} b_{i2}\,. \end{aligned} \tag{10.38}$$

According to (10.29) and (3.49), Student's t pertaining to $\bar{\beta}_1$, is given by

$$T(m-2) = \frac{\bar{\beta}_1 - \mu_{\bar{\beta}_1}}{S\sqrt{\sum_{i=1}^{m} b_{i1}^2}} \tag{10.39}$$

$$= \left(\frac{\bar{\beta}_1 - \mu_{\bar{\beta}_1}}{\sigma\sqrt{\sum_{i=1}^{m} b_{i1}^2}} \right) \left(\frac{S\sqrt{\sum_{i=1}^{m} b_{i1}^2}}{\sigma\sqrt{\sum_{i=1}^{m} b_{i1}^2}} \right)^{-1} = \frac{\left(\bar{\beta}_1 - \mu_{\bar{\beta}_1}\right)/\sigma\sqrt{\sum_{i=1}^{m} b_{i1}^2}}{\sqrt{\frac{\chi^2(m-2)}{m-2}}},$$

where, as usual, S denotes the random variable formally associated with the empirical standard deviation s. Finally, we assign the uncertainties

$$u_{\bar{\beta}_1} = t_P(m-2)s\sqrt{\sum_{i=1}^{m} b_{i1}^2} + f_{s,y}\,; \quad u_{\bar{\beta}_2} = t_P(m-2)s\sqrt{\sum_{i=1}^{m} b_{i2}^2} \tag{10.40}$$

to the components $\bar{\beta}_1, \bar{\beta}_2$ of the solution vector $\bar{\boldsymbol{\beta}}$.

Uncertainty Band

Inserting (10.31) into (10.6) yields

$$\bar{y}(x) = \bar{\beta}_1 + \bar{\beta}_2 x$$

$$= (\beta_{0,1} + \beta_{0,2}x) + \sum_{i=1}^{m} (b_{i1} + b_{i2}x)\,(y_i - \mu_{y_i}) + f_y\,. \tag{10.41}$$

For any fixed x, we subtract the expectation

$$\mu_{\bar{y}(x)} = E\left\{\bar{Y}(x)\right\} = (\beta_{0,1} + \beta_{0,2}x) + f_y \tag{10.42}$$

from (10.41) so that

$$\sigma^2_{\bar{y}(x)} = E\left\{\left(\bar{Y}(x) - \mu_{\bar{y}(x)}\right)^2\right\} = \sigma^2 \sum_{i=1}^{m} (b_{i1} + b_{i2}x)^2\,. \tag{10.43}$$

Obviously, an estimator for $\sigma^2_{\bar{y}(x)}$ is

$$s^2_{\bar{y}(x)} = s^2 \sum_{i=1}^{m} (b_{i1} + b_{i2}x)^2\,. \tag{10.44}$$

Referring to

$$T(m-2) = \frac{\bar{Y}(x) - \mu_{\bar{y}(x)}}{S\sqrt{\sum_{i=1}^{m} (b_{i1} + b_{i2}x)^2}}\,, \tag{10.45}$$

the uncertainty band in question turns out to be

$$\bar{y}(x) \pm u_{\bar{y}(x)}\,; \quad u_{\bar{y}(x)} = t_P(m-2)s\sqrt{\sum_{i=1}^{m}(b_{i1}+b_{i2}x)^2} + f_{s,y}\,. \quad (10.46)$$

Repeat Measurements

Repeat measurements are optional, given that on each of the ordinates one and the same systematic error is superimposed, however, they are indispensable if the ordinates are biased by different systematic errors. The components $\bar{\beta}_1$ and $\bar{\beta}_2$ of the solution vector $\bar{\boldsymbol{\beta}}$ are given in (10.14), the associated coefficients b_{i1} and b_{i2} in (10.19).

Uncertainties of the Components of the Solution Vector

We firstly quote the empirical variance–covariance matrix of the solution vector and the systematic errors of its components. With a view to Fig. 10.1 and the error equations

$$\bar{y}_i = y_{0,i} + (\bar{y}_i - \mu_{\bar{y}_i}) + f_{\bar{y}_i}\,; \quad -f_{s,\bar{y}_i} \le f_{\bar{y}_i} \le f_{s,\bar{y}_i}\,; \quad i = 1,\ldots,m\,,$$

we "expand" the estimators $\bar{\beta}_k$, $k = 1,2$ throughout a neighborhood of the point $(y_{0,1},\ldots,y_{0,2})$,

$$\bar{\beta}_k\,(\bar{y}_1,\ldots,\bar{y}_2) = \bar{\beta}_k\,(y_{0,1},\ldots,y_{0,2}) + \sum_{i=1}^{m}\frac{\partial\bar{\beta}_k}{\partial y_{0,1}}\,(\bar{y}_i - y_{0,i})\,; \quad k = 1,2\,.$$

To abbreviate we set

$$\bar{\beta}_k\,(y_{0,1},\ldots,y_{0,2}) = \beta_{0,k} \quad \text{and} \quad \frac{\partial\bar{\beta}_k}{\partial\bar{y}_{0,i}} = b_{ik}\,.$$

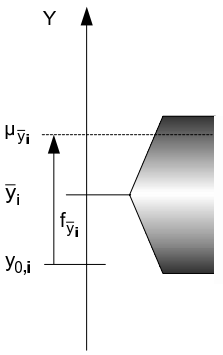


Fig. 10.1. Mean value $\bar{y}_i$, true value $y_{0,i}$, systematic error $f_{\bar{y}_i}$ and expectation $\mu_{\bar{y}_i} = E\{\bar{Y}_i\}$ of the i-th measured ordinate

On the other hand, we could have directly inserted the error equations for $\bar{y}_i$ into (10.14) to find

$$\bar{\beta}_k\left(\bar{y}_1,\ldots,\bar{y}_2\right)=\beta_{0,k}+\sum_{i=1}^{m}b_{ik}\left(\bar{y}_i-\mu_{\bar{y}_i}\right)+\sum_{i=1}^{m}b_{ik}f_{\bar{y}_i}\,;\quad k=1,2\,. \tag{10.47}$$

To assess the second term on the right-hand side, which expresses random errors, we refer to the individual measurements y_{il} via

$$\bar{y}_i=\frac{1}{n}\sum_{l=1}^{n}y_{il}\,;\quad i=1,\ldots,m\,.$$

Hence, (10.14) turns into

$$\bar{\beta}_k=\sum_{i=1}^{m}b_{ik}\left[\frac{1}{n}\sum_{l=1}^{n}y_{il}\right]=\frac{1}{n}\sum_{l=1}^{n}\left[\sum_{i=1}^{m}b_{ik}y_{il}\right]=\frac{1}{n}\sum_{l=1}^{n}\bar{\beta}_{kl}\,;\quad k=1,2 \tag{10.48}$$

where

$$\bar{\beta}_{kl}=\sum_{i=1}^{m}b_{ik}y_{il}\,. \tag{10.49}$$

From (10.14) and (10.49) we obtain

$$\bar{\beta}_{kl}-\bar{\beta}_k=\sum_{i=1}^{m}b_{ik}\left(y_{il}-\bar{y}_i\right)\,. \tag{10.50}$$

Thus, the elements of the empirical variance–covariance matrix of the solution vector take the form

$$\begin{aligned}s_{\bar{\beta}_k\bar{\beta}_{k'}}&=\frac{1}{n-1}\sum_{l=1}^{n}\left(\bar{\beta}_{kl}-\bar{\beta}_k\right)\left(\bar{\beta}_{k'l}-\bar{\beta}_{k'}\right)\\&=\frac{1}{n-1}\sum_{l=1}^{n}\left[\sum_{i=1}^{m}b_{ik}\left(y_{il}-\bar{y}_i\right)\right]\left[\sum_{j=1}^{m}b_{jk'}\left(y_{jl}-\bar{y}_j\right)\right]\\&=\sum_{i,j=1}^{m}b_{ik}b_{jk'}s_{ij}\,;\quad k,k'=1,2\end{aligned} \tag{10.51}$$

in which we recognize the elements

$$s_{ij}=\frac{1}{n-1}\sum_{l=1}^{n}\left(y_{il}-\bar{y}_i\right)\left(y_{jl}-\bar{y}_j\right)\,;\quad i,j=1,\ldots,m \tag{10.52}$$

of the empirical variance–covariance matrix s of the input data. Finally, we denote

$$\boldsymbol{s}_{\bar{\beta}} = \begin{pmatrix} s_{\bar{\beta}_1\bar{\beta}_1} & s_{\bar{\beta}_1\bar{\beta}_2} \\ s_{\bar{\beta}_2\bar{\beta}_1} & s_{\bar{\beta}_2\bar{\beta}_2} \end{pmatrix} = \boldsymbol{B}^{\mathrm{T}} \boldsymbol{s}\, \boldsymbol{B}\,; \quad s_{\bar{\beta}_k\bar{\beta}_k} \equiv s^2_{\bar{\beta}_k}\,. \tag{10.53}$$

According to (10.48) and (10.49), the $\bar{\beta}_k$ are the arithmetic means of n independent, normally distributed quantities $\bar{\beta}_{kl}$. Consequently, we may define Student's confidence intervals

$$\bar{\beta}_k - \frac{t_P(n-1)}{\sqrt{n}} s_{\bar{\beta}_k} \le \mu_{\bar{\beta}_k} \le \bar{\beta}_k + \frac{t_P(n-1)}{\sqrt{n}} s_{\bar{\beta}_k}\,; \quad k = 1, 2 \tag{10.54}$$

for the expectations $E\{\bar{\beta}_k\} = \mu_{\bar{\beta}_k}; k = 1, 2$. The propagated systematic errors follow from (10.47). Their worst case estimations turn out to be

$$f_{s,\bar{\beta}_k} = \sum_{i=1}^{m} |b_{ik}|\, f_{s,\bar{y}_i}\,; \quad k = 1, 2\,. \tag{10.55}$$

Finally, the overall uncertainties $u_{\bar{\beta}_k}$ of the estimators $\bar{\beta}_k \pm u_{\bar{\beta}_k}$, $k = 1, 2$ are given by

$$\begin{aligned} u_{\bar{\beta}_k} &= \frac{t_P(n-1)}{\sqrt{n}} s_{\bar{\beta}_k} + f_{s,\bar{\beta}_k} \\ &= \frac{t_P(n-1)}{\sqrt{n}} \sqrt{\sum_{i,j=1}^{m} b_{ik} b_{jk} s_{ij}} + \sum_{i=1}^{m} |b_{ik}|\, f_{s,\bar{y}_i}\,; \quad k = 1, 2\,. \end{aligned} \tag{10.56}$$

Equal Systematic Errors

Let $f_{\bar{y}_i} = f_y$, $f_{s,\bar{y}_i} = f_{s,y}$; $i = 1, \ldots, m$. From (10.47) we then deduce

$$f_{\bar{\beta}_k} = \sum_{i=1}^{m} b_{ik} f_{\bar{y}_i} = f_y \sum_{i=1}^{m} b_{ik}\,. \tag{10.57}$$

Because of (10.32) we have

$$f_{\bar{\beta}_1} = f_y\,; \quad f_{\bar{\beta}_2} = 0 \tag{10.58}$$

so that

$$\begin{aligned} u_{\bar{\beta}_1} &= \frac{t_P(n-1)}{\sqrt{n}} \sqrt{\sum_{i,j=1}^{m} b_{i1} b_{j1} s_{ij}} + f_{s,y} \\ u_{\bar{\beta}_2} &= \frac{t_P(n-1)}{\sqrt{n}} \sqrt{\sum_{i,j=1}^{m} b_{i2} b_{j2} s_{ij}}\,. \end{aligned} \tag{10.59}$$

Uncertainty Band

As disclosed through (10.14) and (10.56), it clearly is not only a single straight line which is compatible with the input data and the error model. Rather, in addition to (10.6), arbitrary many least squares lines would apply just as well. Speaking vividly, what we expect is something like the "bow net" shaped uncertainty band similar to (10.46). Inserting (10.47),

$$\bar{\beta}_k\,(\bar{y}_1,\ldots,\bar{y}_2) = \beta_{0,k} + \sum_{i=1}^{m} b_{ik}\,(\bar{y}_i - \mu_{\bar{y}_i}) + \sum_{i=1}^{m} b_{ik} f_{\bar{y}_i}\,; \quad k = 1,2$$

into (10.6),

$$\bar{y}(x) = \bar{\beta}_1 + \bar{\beta}_2 x\,,$$

yields

$$\bar{y}(x) = \beta_{0,1} + \beta_{0,2}x + \sum_{i=1}^{m} (b_{i1} + b_{i2}x)\,(\bar{y}_i - \mu_{\bar{y}_i}) + \sum_{i=1}^{m} (b_{i1} + b_{i2}x)\, f_{\bar{y}_i}\,. \tag{10.60}$$

We first estimate the contribution due to random errors. To this end, we insert (10.48),

$$\bar{\beta}_k = \frac{1}{n}\sum_{l=1}^{n} \bar{\beta}_{kl}\,; \qquad k = 1,2\,,$$

into (10.6)

$$\begin{aligned}\bar{y}(x) &= \frac{1}{n}\sum_{l=1}^{n} \bar{\beta}_{1l} + \frac{1}{n}\sum_{l=1}^{n} \bar{\beta}_{2l} x \\ &= \frac{1}{n}\sum_{l=1}^{n} \left(\bar{\beta}_{1l} + \bar{\beta}_{2l} x\right) = \frac{1}{n}\sum_{l=1}^{n} \bar{y}_l(x)\,. \end{aligned} \tag{10.61}$$

Obviously,

$$\bar{y}_l(x) = \bar{\beta}_{1l} + \bar{\beta}_{2l} x\,; \quad l = 1,\ldots,n \tag{10.62}$$

designates a fitted line which we would get if at every i-th measuring point we inserted just the l-th measured value y_{il}. Referring to (10.49) and to (10.14), we have

$$\bar{\beta}_{kl} = \sum_{i=1}^{m} b_{ik} y_{il}\,, \quad l = 1,\ldots,n \quad \text{and} \quad \bar{\beta}_k = \sum_{i=1}^{m} b_{ik}\bar{y}_i\,.$$

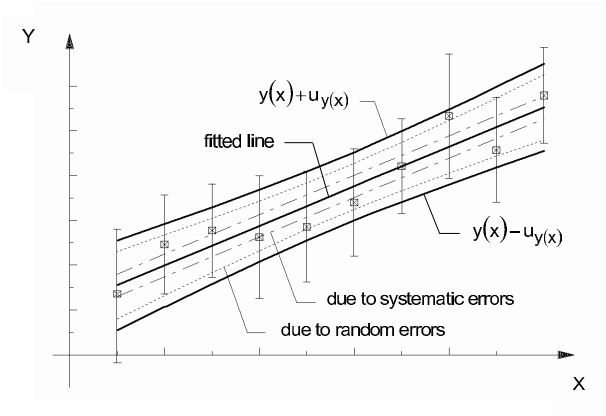


Fig. 10.2. Measuring points, measurement uncertainties, least squares fit and "bow net" shaped uncertainty band

Then, for any fixed x, the difference

$$\begin{aligned}\bar{y}_l(x) - \bar{y}(x) &= \left(\bar{\beta}_{1l} - \bar{\beta}_1\right) + \left(\bar{\beta}_{2l} - \bar{\beta}_2\right) x \\ &= \sum_{i=1}^{m} \left(b_{i1} + b_{i2} x\right) \left(y_{il} - \bar{y}_i\right) \end{aligned} \tag{10.63}$$

gives rise to an empirical variance

$$s^2_{\bar{y}(x)} = \frac{1}{n-1} \sum_{l=1}^{n} \left[\bar{y}_l(x) - \bar{y}(x)\right]^2 = \boldsymbol{b}^{\mathrm{T}} \boldsymbol{s} \boldsymbol{b}\,, \tag{10.64}$$

where for convenience the auxiliary vector

$$\boldsymbol{b} = \left(b_{11} + b_{12} x \quad b_{21} + b_{22} x \quad \ldots \quad b_{m1} + b_{m2} x\right)^{\mathrm{T}} \tag{10.65}$$

has been introduced. According to (10.60), the propagated systematic error is given by

$$f_{\bar{y}(x)} = \sum_{i=1}^{m} \left(b_{i1} + b_{i2} x\right) f_{\bar{y}_i}\,, \tag{10.66}$$

and its worst case estimate is

$$f_{s,\bar{y}(x)} = \sum_{i=1}^{m} \left|b_{i1} + b_{i2} x\right| f_{s,\bar{y}_i}\,. \tag{10.67}$$

As shown in Fig. 10.2, for any fixed x, the uncertainty $u_{y(x)}$ of the least squares fit (10.6),

$$\bar{y}(x) = \bar{\beta}_1 + \bar{\beta}_2 x\,,$$

takes the form

$$\begin{aligned} u_{\bar{y}(x)} &= \frac{t_P(n-1)}{\sqrt{n}} s_{y(x)} + f_{s,y(x)} \\ &= \frac{t_P(n-1)}{\sqrt{n}} \sqrt{\boldsymbol{b}^{\mathrm{T}} \boldsymbol{s}\, \boldsymbol{b}} + \sum_{i=1}^{m} |b_{i1} + b_{i2} x|\, f_{s,\bar{y}_i}\,. \end{aligned} \tag{10.68}$$

Hence, the true straight line (10.4),

$$y_0(x) = \beta_{0,1} + \beta_{0,2} x\,,$$

should lie within the uncertainty band

$$\bar{y}(x) \pm u_{\bar{y}(x)}\,. \tag{10.69}$$

Equal Systematic Errors

Let $f_{\bar{y}_i} = f_y$, $f_{s,\bar{y}_i} = f_{s,y}$; $i = 1, \ldots, m$. Because of (10.32), the relationship (10.66) turns into

$$f_{\bar{y}(x)} = f_y \sum_{i=1}^{m} (b_{i1} + b_{i2} x) = f_y\,, \tag{10.70}$$

i.e.

$$u_{\bar{y}(x)} = \frac{t_P(n-1)}{\sqrt{n}} s_{\bar{y}(x)} + f_{s,y} = \frac{t_P(n-1)}{\sqrt{n}} \sqrt{\boldsymbol{b}^{\mathrm{T}} \boldsymbol{s}\, \boldsymbol{b}} + f_{s,y}\,. \tag{10.71}$$

To check this, we compare (10.56) with (10.68) for the special case $\bar{y}(0) = \bar{\beta}_1$. The uncertainty $u_{\bar{\beta}_1}$ should be equal to the uncertainty $u_{y(x)}$ in $x = 0$. If $x = 0$, the vector $\boldsymbol{b}$ as defined in (10.65) turns out to be

$$\boldsymbol{b}_1 = (b_{11} \quad b_{21} \quad \ldots \quad b_{m1})^{\mathrm{T}}\,;$$

hence

$$s^2_{\bar{y}(0)} = s_{\bar{\beta}_1 \bar{\beta}_1} \equiv s^2_{\bar{\beta}_1} \tag{10.72}$$

so that

$$u_{\bar{y}(0)} = \frac{t_P(n-1)}{\sqrt{n}} s_{\bar{\beta}_1} + \sum_{i=1}^{m} |b_{i1}|\, f_{s,\bar{y}_i} \tag{10.73}$$

which agrees with (10.56).

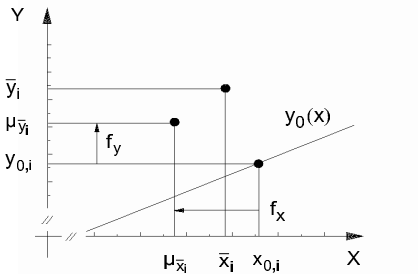


Fig. 10.3. Measuring points $(\bar{x}_i, \bar{y}_i)$, expectations $(\mu_{\bar{x}_i}, \mu_{\bar{y}_i})$ and true values $(x_{0,i}, y_{0,i})$

10.1.2 Erroneous Abscissas, Erroneous Ordinates

It would be more realistic to consider both coordinates, the abscissas and the ordinates, to be affected by measurement errors, Fig. 10.3.

Uncertainties of the Components of the Solution Vector

Let us expand the elements b_{ik} of the matrix $\boldsymbol{B}$ as defined in (10.17). Indeed, under the conditions considered, these elements are erroneous so that, in contrast to (10.47), now there is no other choice,

$$\bar{\beta}_k\,(\bar{x}_1, \ldots, \bar{y}_m) = \bar{\beta}_k\,(x_{0,1}, \ldots, y_{0,m}) + \sum_{i=1}^{m} \frac{\partial \bar{\beta}_k}{\partial x_{0,i}}\,(\bar{x}_i - x_{0,i}) + \sum_{i=1}^{m} \frac{\partial \bar{\beta}_k}{\partial y_{0,i}}\,(\bar{y}_i - y_{0,i}) + \cdots \tag{10.74}$$

Linearizing the expansion, approximating the derivatives in $(x_{0,1}, \ldots, y_{0,m})$ through derivatives in $(\bar{x}_1, \ldots, \bar{y}_m)$ and inserting the error equations

$$\bar{x}_i = x_{0,i} + (\bar{x}_i - \mu_{\bar{x}_i}) + f_{\bar{x}_i}\,; \quad -f_{s,\bar{x}_i} \le f_{\bar{x}_i} \le f_{s,\bar{x}_i}$$
$$\bar{y}_i = y_{0,i} + (\bar{y}_i - \mu_{\bar{y}_i}) + f_{\bar{y}_i}\,; \quad -f_{s,\bar{y}_i} \le f_{\bar{y}_i} \le f_{s,\bar{y}_i}$$

yields, as $\bar{\beta}_k(x_{0,1}, \ldots, y_{0,m}) = \beta_{0,k}$,

$$\bar{\beta}_1\,(\bar{x}_1, \ldots, \bar{y}_m) = \beta_{0,1} + \sum_{i=1}^{m} \frac{\partial \bar{\beta}_1}{\partial \bar{x}_i}\,(\bar{x}_i - \mu_{\bar{x}_i}) + \sum_{i=1}^{m} \frac{\partial \bar{\beta}_1}{\partial \bar{y}_i}\,(\bar{y}_i - \mu_{\bar{y}_i}) + \sum_{i=1}^{m} \frac{\partial \bar{\beta}_1}{\partial \bar{x}_i} f_{\bar{x}_i} + \sum_{i=1}^{m} \frac{\partial \bar{\beta}_1}{\partial \bar{y}_i} f_{\bar{y}_i} \tag{10.75}$$

and

$$\bar{\beta}_2\,(\bar{x}_1, \ldots, \bar{y}_m) = \beta_{0,2} + \sum_{i=1}^{m} \frac{\partial \bar{\beta}_2}{\partial \bar{x}_i}\,(\bar{x}_i - \mu_{\bar{x}_i}) + \sum_{i=1}^{m} \frac{\partial \bar{\beta}_2}{\partial \bar{y}_i}\,(\bar{y}_i - \mu_{\bar{y}_i}) + \sum_{i=1}^{m} \frac{\partial \bar{\beta}_2}{\partial \bar{x}_i} f_{\bar{x}_i} + \sum_{i=1}^{m} \frac{\partial \bar{\beta}_2}{\partial \bar{y}_i} f_{\bar{y}_i}\,. \tag{10.76}$$

To establish the partial derivatives, we insert (10.18) into (10.14),

$$\begin{aligned}\bar{\beta}_1 &= \sum_{i=1}^{m} b_{i1}\bar{y}_i \\ &= \frac{1}{D}\sum_{i=1}^{m}\left[\sum_{j=1}^{m}\bar{x}_j^2 - \bar{x}_i\sum_{j=1}^{m}\bar{x}_j\right]\bar{y}_i = \frac{1}{D}\left[\sum_{j=1}^{m}\bar{y}_j\sum_{j=1}^{m}\bar{x}_j^2 - \sum_{j=1}^{m}\bar{x}_j\bar{y}_j\sum_{j=1}^{m}\bar{x}_j\right]\end{aligned}$$

so that

$$\frac{\partial\bar{\beta}_1}{\partial\bar{x}_i} = \frac{1}{D}\left[2\bar{x}_i\sum_{j=1}^{m}\bar{y}_j - \bar{y}_i\sum_{j=1}^{m}\bar{x}_j - \sum_{j=1}^{m}\bar{x}_j\bar{y}_j\right] - \frac{2\bar{\beta}_1}{D}\left[m\bar{x}_i - \sum_{j=1}^{m}\bar{x}_j\right] \quad (10.77)$$

and

$$\frac{\partial\bar{\beta}_1}{\partial\bar{y}_i} = b_{i1} = \frac{1}{D}\left[\sum_{j=1}^{m}\bar{x}_j^2 - \bar{x}_i\sum_{j=1}^{m}\bar{x}_j\right]. \quad (10.78)$$

Similarly, from

$$\begin{aligned}\bar{\beta}_2 &= \sum_{i=1}^{m} b_{i2}\bar{y}_i \\ &= \frac{1}{D}\sum_{i=1}^{m}\left[-\sum_{j=1}^{m}\bar{x}_j + m\bar{x}_i\right]\bar{y}_i = \frac{1}{D}\left[-\sum_{j=1}^{m}\bar{x}_j\sum_{j=1}^{m}\bar{y}_j + m\sum_{j=1}^{m}\bar{x}_j\bar{y}_j\right]\end{aligned}$$

we obtain

$$\frac{\partial\bar{\beta}_2}{\partial\bar{x}_i} = \frac{1}{D}\left[-\sum_{j=1}^{m}\bar{y}_j + m\bar{y}_i\right] - \frac{2\bar{\beta}_2}{D}\left[m\bar{x}_i - \sum_{j=1}^{m}\bar{x}_j\right] \quad (10.79)$$

and

$$\frac{\partial\bar{\beta}_2}{\partial\bar{y}_i} = b_{i2} = \frac{1}{D}\left[-\sum_{j=1}^{m}\bar{x}_j + m\bar{x}_i\right]. \quad (10.80)$$

In (10.75) and (10.76), random and systematic errors are each expressed through two terms. Let us repeat the expansions of $\bar{\beta}_1$ and $\bar{\beta}_2$, this time, however, throughout a neighborhood of the point

$$(\bar{x}_1, \ldots, \bar{x}_m; \bar{y}_1, \ldots, \bar{y}_m)$$

and with respect to the l-th repeat measurements of the measuring points $i = 1, \ldots, m$, i.e. with respect to the data set

$$(x_{1l},\dots,x_{ml};y_{1l},\dots,y_{ml})\;;\quad l=1,\dots,n\,.$$

We then find

$$\begin{aligned}\bar\beta_{1l}\,(x_{1l},\dots,x_{ml};y_{1l},\dots,y_{ml}) &= \bar\beta_1\,(\bar x_1,\dots,\bar x_m;\bar y_1,\dots,\bar y_m)\\ &+\sum_{i=1}^{m}\frac{\partial\bar\beta_1}{\partial\bar x_i}\,(x_{il}-\bar x_i)+\sum_{i=1}^{m}\frac{\partial\bar\beta_1}{\partial\bar y_i}\,(y_{il}-\bar y_i)+\cdots\end{aligned}\tag{10.81}$$

and

$$\begin{aligned}\bar\beta_{2l}\,(x_{1l},\dots,x_{ml};y_{1l},\dots,y_{ml}) &= \bar\beta_2\,(\bar x_1,\dots,\bar x_m;\bar y_1,\dots,\bar y_m)\\ &+\sum_{i=1}^{m}\frac{\partial\bar\beta_2}{\partial\bar x_i}\,(x_{il}-\bar x_i)+\sum_{i=1}^{m}\frac{\partial\bar\beta_2}{\partial\bar y_i}\,(y_{il}-\bar y_i)+\cdots\,.\end{aligned}\tag{10.82}$$

Obviously, the linearizations imply

$$\bar\beta_k=\frac{1}{n}\sum_{l=1}^{n}\beta_{kl}\;;\quad k=1,2\,.$$

For convenience, we simplify the nomenclature by introducing the definitions

$$\begin{aligned} v_{il}&=x_{il}\,, & v_{i+m,l}&=y_{il}\\ \bar v_i&=\bar x_i\,, & \bar v_{i+m}&=\bar y_i\\ \mu_i&=\mu_{\bar x_i}\,, & \mu_{i+m}&=\mu_{\bar y_i}\\ f_i&=f_{\bar x_i}\,, & f_{i+m}&=f_{\bar y_i}\\ f_{s,i}&=f_{s,\bar x_i}\,, & f_{s,i+m}&=f_{s,\bar y_i}\end{aligned}\tag{10.83}$$

and

$$\begin{aligned} c_{i1}&=\frac{\partial\bar\beta_1}{\partial\bar x_i}\,, & c_{i+m,1}&=\frac{\partial\bar\beta_1}{\partial\bar y_i}\\ c_{i2}&=\frac{\partial\bar\beta_2}{\partial\bar x_i}\,, & c_{i+m,2}&=\frac{\partial\bar\beta_2}{\partial\bar y_i}\,.\end{aligned}\tag{10.84}$$

Applying this notation, the expansions (10.75), (10.76), (10.81) and (10.82) turn into

$$\bar\beta_k=\beta_{0,k}+\sum_{i=1}^{2m}c_{ik}\,(\bar v_i-\mu_i)+\sum_{i=1}^{2m}c_{ik}f_i\;;\quad k=1,2\tag{10.85}$$

and

$$\bar\beta_{kl}-\bar\beta_k=\sum_{i=1}^{2m}c_{ik}\,(v_{il}-\bar v_i)\;;\quad k=1,2\,.\tag{10.86}$$

From (10.86) we deduce the elements

$$\begin{aligned} s_{\bar{\beta}_k\bar{\beta}_{k'}} &= \frac{1}{n-1}\sum_{l=1}^{n}\left(\bar{\beta}_{kl}-\bar{\beta}_k\right)\left(\bar{\beta}_{k'l}-\bar{\beta}_{k'}\right) \\ &= \frac{1}{n-1}\sum_{l=1}^{n}\left[\sum_{i=1}^{2m} c_{ik}\left(v_{il}-\bar{v}_i\right)\right]\left[\sum_{j=1}^{2m} c_{jk'}\left(v_{jl}-\bar{v}_j\right)\right] \\ &= \sum_{i,j=1}^{2m} c_{ik}c_{jk'}s_{ij} \end{aligned} \tag{10.87}$$

of the empirical variance–covariance matrix $\boldsymbol{s}_{\bar{\boldsymbol{\beta}}}$ of the solution vector, in which the

$$s_{ij} = \frac{1}{n-1}\sum_{l=1}^{n}\left(v_{il}-\bar{v}_i\right)\left(v_{jl}-\bar{v}_j\right)\,; \quad i,j=1,\ldots,2m$$

designate the elements of the (expanded) empirical variance–covariance matrix

$$\boldsymbol{s} = (s_{ij})$$

of the input data. We condense the coefficients c_{i1} and c_{i2} into the auxiliary matrix

$$\boldsymbol{C}^{\mathrm{T}} = \begin{pmatrix} c_{11}\ c_{21}\ \cdots\ c_{2m,1} \\ c_{12}\ c_{22}\ \cdots\ c_{2m,2} \end{pmatrix}$$

and arrive, in analogy to (10.53), at

$$\boldsymbol{s}_{\bar{\boldsymbol{\beta}}} = \begin{pmatrix} s_{\bar{\beta}_1\bar{\beta}_1}\ s_{\bar{\beta}_1\bar{\beta}_2} \\ s_{\bar{\beta}_2\bar{\beta}_1}\ s_{\bar{\beta}_2\bar{\beta}_2} \end{pmatrix} = \boldsymbol{C}^{\mathrm{T}}\boldsymbol{s}\boldsymbol{C}\,; \quad s_{\bar{\beta}_k\bar{\beta}_k} \equiv s^2_{\bar{\beta}_k}\,. \tag{10.88}$$

Finally, in view of (10.85) and (10.87), we may assign the uncertainties

$$u_{\bar{\beta}_k} = \frac{t_P(n-1)}{\sqrt{n}}\sqrt{\sum_{i,j=1}^{2m} c_{ik}c_{jk}s_{ij}} + \sum_{i=1}^{2m}\left|c_{ik}\right| f_{s,i}\,; \quad k=1,2 \tag{10.89}$$

to the estimators $\bar{\beta}_k \pm u_{\bar{\beta}_k}$, $k=1,2$.

Equal Systematic Errors

Let $f_{\bar{x}_i} = f_x$, $f_{s,\bar{x}_i} = f_{s,x}$; $f_{\bar{y}_i} = f_y$, $f_{s,\bar{y}_i} = f_{s,y}$; $i=1,\ldots,m$. From (10.75) we obtain

$$\sum_{i=1}^{m} \frac{\partial \bar{\beta}_1}{\partial \bar{x}_i} f_{\bar{x}_i} + \sum_{i=1}^{m} \frac{\partial \bar{\beta}_1}{\partial \bar{y}_i} f_{\bar{y}_i} = f_x \sum_{i=1}^{m} c_{i1} + f_y \sum_{i=1}^{m} c_{i+m,1} = -f_x \bar{\beta}_2 + f_y$$

and from (10.76)

$$\sum_{i=1}^{m} \frac{\partial \bar{\beta}_2}{\partial \bar{x}_i} f_{\bar{x}_i} + \sum_{i=1}^{m} \frac{\partial \bar{\beta}_2}{\partial \bar{y}_i} f_{\bar{y}_i} = f_x \sum_{i=1}^{m} c_{i2} + f_y \sum_{i=1}^{m} c_{i+m,2} = 0\,.$$

Hence, (10.89) turns into

$$u_{\bar{\beta}_1} = \frac{t_P(n-1)}{\sqrt{n}} \sqrt{\sum_{i,j=1}^{2m} c_{i1} c_{j1} s_{ij}} + f_{s,x} \left|\bar{\beta}_2\right| + f_{s,y} \tag{10.90}$$

and

$$u_{\bar{\beta}_2} = \frac{t_P(n-1)}{\sqrt{n}} \sqrt{\sum_{i,j=1}^{2m} c_{i2} c_{j2} s_{ij}}\,. \tag{10.91}$$

Uncertainty Band

Inserting (10.85) into the fitted line $\bar{y}(x) = \bar{\beta}_1 + \bar{\beta}_2 x$, we obtain

$$\begin{aligned} \bar{y}(x) = \beta_{0,1} + \beta_{0,2} x &+ \sum_{i=1}^{2m} (c_{i1} + c_{i2} x)\,(\bar{v}_i - \mu_i) \\ &+ \sum_{i=1}^{2m} (c_{i1} + c_{i2} x)\, f_i\,. \end{aligned} \tag{10.92}$$

To estimate the contribution due to random errors we refer to the n least squares lines of the repeat measurements,

$$\bar{y}_l(x) = \bar{\beta}_{1l} + \bar{\beta}_{2l} x\,; \quad l = 1, \ldots, n\,.$$

Upon insertion of (10.86), the difference

$$\bar{y}_l(x) - \bar{y}(x) = \left(\bar{\beta}_{1l} - \bar{\beta}_1\right) + \left(\bar{\beta}_{2l} - \bar{\beta}_2\right) x\,; \quad l = 1, \ldots, n \tag{10.93}$$

changes into

$$\bar{y}_l(x) - \bar{y}(x) = \sum_{i=1}^{2m} (c_{i1} + c_{i2} x)\,(v_{il} - \bar{v}_i)\;; \quad l = 1, \ldots, n \tag{10.94}$$

so that

$$s^2_{\bar{y}(x)} = \boldsymbol{c}^{\mathrm{T}} \boldsymbol{s} \boldsymbol{c} \tag{10.95}$$

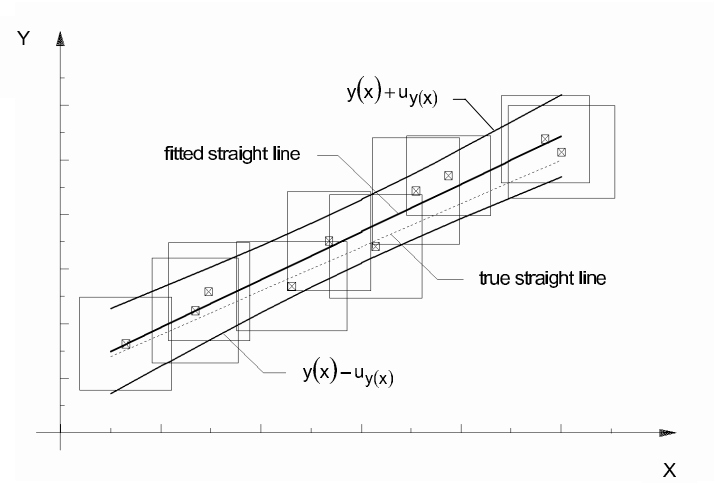


Fig. 10.4. Measuring points, uncertainty rectangles, fitted straight line, "bow net" shaped uncertainty band and true straight line

where for convenience the auxiliary vector

$$\boldsymbol{c} = (c_{11} + c_{12}x \quad c_{21} + c_{22}x \quad \cdots \quad c_{2m,1} + c_{2m,2}x)^{\mathrm{T}}$$

has been introduced. As (10.92) shows, the propagated systematic error is given by

$$f_{\bar{y}(x)} = \sum_{i=1}^{2m} (c_{i1} + c_{i2}x)\, f_i\,. \tag{10.96}$$

Its worst case estimation yields

$$f_{s,\bar{y}(x)} = \sum_{i=1}^{2m} |c_{i1} + c_{i2}x|\, f_{s,i}\,. \tag{10.97}$$

As illustrated in Fig. 10.4, the "bow net" shaped uncertainty band takes the form

$$\bar{y}(x) \pm u_{\bar{y}(x)} \tag{10.98}$$

$$u_{\bar{y}(x)} = \frac{t_P(n-1)}{\sqrt{n}} s_{\bar{y}(x)} + f_{s,\bar{y}(x)} = \frac{t_P(n-1)}{\sqrt{n}} \sqrt{\boldsymbol{c}^{\mathrm{T}} \boldsymbol{s} \boldsymbol{c}} + \sum_{i=1}^{2m} |c_{i1} + c_{i2}x|\, f_{s,i}\,.$$

Equal Systematic Errors

Let $f_{\bar{x}_i} = f_x$, $f_{s,\bar{x}_i} = f_{s,x}$; $f_{\bar{y}_i} = f_y$, $f_{s,\bar{y}_i} = f_{s,y}$; $i = 1, \ldots, m$. Then, from (10.96) we deduce

$$f_{\bar{y}(x)} = -f_x \bar{\beta}_2 + f_y \,, \tag{10.99}$$

the worst case estimation is

$$f_{s,\bar{y}(x)} = f_{s,x} \left|\bar{\beta}_2\right| + f_{s,y} \,. \tag{10.100}$$

The modified overall uncertainty is given by

$$u_{\bar{y}(x)} = \frac{t_P(n-1)}{\sqrt{n}} \sqrt{\boldsymbol{c}^{\mathrm{T}} \boldsymbol{s} \boldsymbol{c}} + f_{s,x} \left|\bar{\beta}_2\right| + f_{s,y} \,. \tag{10.101}$$

Again, we may convince ourselves that $u_{\bar{y}(0)} = u_{\bar{\beta}_1}$.

Example

Measurement of the linear coefficient of expansion. The length $L(t)$ of a rod is to be measured with respect to the temperature t. Let α denote the linear coefficient of expansion. Then we have

$$L(t) = L_{\mathrm{r}} \left[1 + \alpha \left(t - t_{\mathrm{r}}\right)\right] = L_{\mathrm{r}} + \alpha L_{\mathrm{r}} \left(t - t_{\mathrm{r}}\right) \,.$$

Here, L_{r} denotes the length of the rod at some reference temperature t_{r}. Setting $x = t - t_{\mathrm{r}}$, $y = L(t)$, $\beta_1 = L_{\mathrm{r}}$, and $\beta_2 = \alpha L_{\mathrm{r}}$, we obtain

$$y(x) = \beta_1 + \beta_2 x \,.$$

The uncertainties $u_{\bar{\beta}_1}$, $u_{\bar{\beta}_2}$ have already been quoted in (10.89). Consequently, we may confine ourselves to assessing the uncertainty $u_{\bar{\alpha}}$ of the coefficient

$$\bar{\alpha} = \phi\left(\bar{\beta}_1, \bar{\beta}_2\right) = \bar{\beta}_2 / \bar{\beta}_1 \,,$$

see Sect. 9.4. Inserting (10.85),

$$\bar{\beta}_k = \beta_{0,k} + \sum_{i=1}^{2m} c_{ik} \left(\bar{v}_i - \mu_i\right) + \sum_{i=1}^{2m} c_{ik} f_i \,; \quad k = 1, 2$$

into the expansion

$$\phi\left(\bar{\beta}_1, \bar{\beta}_2\right) = \phi\left(\bar{\beta}_{0,1}, \bar{\beta}_{0,2}\right) + \frac{\partial \phi}{\partial \beta_{0,1}} \left(\bar{\beta}_1 - \beta_{0,1}\right) + \frac{\partial \phi}{\partial \beta_{0,2}} \left(\bar{\beta}_2 - \beta_{0,2}\right) + \cdots$$

yields

$$\begin{aligned} \phi\left(\bar{\beta}_1, \bar{\beta}_2\right) = \phi\left(\bar{\beta}_{0,1}, \bar{\beta}_{0,2}\right) &+ \sum_{i=1}^{2m} \left(\frac{\partial \phi}{\partial \bar{\beta}_1} c_{i1} + \frac{\partial \phi}{\partial \bar{\beta}_2} c_{i2} \right) \left(\bar{v}_i - \mu_i\right) \\ &+ \sum_{i=1}^{2m} \left(\frac{\partial \phi}{\partial \bar{\beta}_1} c_{i1} + \frac{\partial \phi}{\partial \bar{\beta}_2} c_{i2} \right) f_i \,, \end{aligned}$$

where the partial derivatives are given by

$$\frac{\partial\phi}{\partial\bar{\beta}_1} \approx -\frac{\bar{\alpha}}{\bar{\beta}_1}\,; \quad \frac{\partial\phi}{\partial\bar{\beta}_2} \approx \frac{1}{\bar{\beta}_1}\,.$$

Further expansion with respect to $\bar{\beta}_{1l}$ and $\bar{\beta}_{2l}$ leads to

$$\phi\left(\bar{\beta}_{1l},\bar{\beta}_{2l}\right) = \phi\left(\bar{\beta}_1,\bar{\beta}_2\right) + \frac{\partial\phi}{\partial\bar{\beta}_1}\left(\bar{\beta}_{1l}-\bar{\beta}_1\right) + \frac{\partial\phi}{\partial\bar{\beta}_2}\left(\bar{\beta}_{2l}-\bar{\beta}_2\right)$$

so that

$$\begin{aligned} s_{\bar{\phi}}^2 &= \frac{1}{n-1}\sum_{l=1}^{n}\left[\phi\left(\bar{\beta}_{1l},\bar{\beta}_{2l}\right) - \phi\left(\bar{\beta}_1,\bar{\beta}_2\right)\right]^2 \\ &= \left(\frac{\partial\phi}{\partial\bar{\beta}_1}\right)^2 s_{\bar{\beta}_1\bar{\beta}_1} + 2\left(\frac{\partial\phi}{\partial\bar{\beta}_1}\frac{\partial\phi}{\partial\bar{\beta}_2}\right) s_{\bar{\beta}_1\bar{\beta}_2} + \left(\frac{\partial\phi}{\partial\bar{\beta}_2}\right)^2 s_{\bar{\beta}_2\bar{\beta}_2}\,. \end{aligned}$$

Hence, the uncertainty $u_{\bar{\alpha}}$ of the result $\bar{\alpha} \pm u_{\bar{\alpha}}$ follows from

$$\begin{aligned} u_{\bar{\alpha}} = \frac{t_P(n-1)}{\sqrt{n}}&\sqrt{\left(\frac{\partial\phi}{\partial\bar{\beta}_1}\right)^2 s_{\bar{\beta}_1\bar{\beta}_1} + 2\left(\frac{\partial\phi}{\partial\bar{\beta}_1}\frac{\partial\phi}{\partial\bar{\beta}_2}\right) s_{\bar{\beta}_1\bar{\beta}_2} + \left(\frac{\partial\phi}{\partial\bar{\beta}_2}\right)^2 s_{\bar{\beta}_2\bar{\beta}_2}} \\ &+ \sum_{i=1}^{2m}\left|\frac{\partial\phi}{\partial\bar{\beta}_1}c_{i1} + \frac{\partial\phi}{\partial\bar{\beta}_2}c_{i2}\right| f_{s,i}\,. \end{aligned}$$

10.2 Linearization

Let $\phi(x,y;a,b) = 0$ be some non-linear function whose parameters a and b are to be estimated by means of m measured data pairs $(\bar{x}_i,\bar{y}_i)$; $i = 1,\ldots,m$. In order to linearize the function through series expansion and subsequent truncation, we have to assume that estimates or starting values a^*, b^* exist. The series expansion yields

$$\begin{aligned} &\phi(x,y;\,a,b) = \phi(x,y;\,a^*,b^*) \\ &+\frac{\partial\phi(x,y;\,a^*,b^*)}{\partial a^*}\left(a-a^*\right) + \frac{\partial\phi\left(x,y;\,a^*,b*\right)}{\partial b^*}\left(b-b^*\right) + \cdots \end{aligned} \tag{10.102}$$

Clearly, the closer the estimates a^*, b^* to the true values a_0, b_0, the smaller the linearization errors. Considering the differences

$$\beta_1 = a - a^* \quad \text{and} \quad \beta_2 = b - b^* \tag{10.103}$$

as unknowns and setting

$$\bar{u}_i = \frac{\dfrac{\partial\phi\left(\bar{x}_i,\bar{y}_i\,;a^*,b^*\right)}{\partial b^*}}{\dfrac{\partial\phi\left(\bar{x}_i,\bar{y}_i;\,a^*,b^*\right)}{\partial a^*}}\,, \quad \bar{v}_i = -\frac{\phi\left(\bar{x}_i,\bar{y}_i;\,a^*,b^*\right)}{\dfrac{\partial\phi\left(\bar{x}_i,\bar{y}_i;\,a^*,b^*\right)}{\partial a^*}}\,, \tag{10.104}$$

relation (10.102) turns into

$$\beta_1 + \beta_2 \bar{u}_i \approx \bar{v}_i \,; \quad i = 1, \ldots, m \,. \tag{10.105}$$

The least squares estimators $\bar{\beta}_1$ and $\bar{\beta}_2$ lead to the quantities

$$a = a^* + \beta_1 \quad \text{and} \quad b = b^* + \beta_2 \tag{10.106}$$

which, given the procedure converges, will be closer to the true values a_0, b_0 than the starting values a^*, b^*. In this case we shall cyclically repeat the adjustment until

$$\bar{\beta}_1 \approx 0 \quad \text{and} \quad \bar{\beta}_2 \approx 0 \,. \tag{10.107}$$

If the input data were error free, the cycles would reduce the estimators $\bar{\beta}_1, \bar{\beta}_2$ down to the numerical uncertainty of the computer. However, as the input data are erroneous, after a certain number of cycles, the numerical values of the estimators $\bar{\beta}_1, \bar{\beta}_2$ will start to oscillate around some residuals which are different from zero and reflect the degree of accuracy of the input data.

The uncertainties of the estimators $\bar{\beta}_1, \bar{\beta}_2$ pass to the uncertainties of the parameters a and b according to

$$u_{\bar{\beta}_1} = u_a \,; \quad u_{\bar{\beta}_2} = u_b \tag{10.108}$$

as the quantities a^*, b^* enter error-free. The estimation of the uncertainties $u_{\bar{\beta}_1}$, $u_{\bar{\beta}_2}$ has been explained in Sect. 10.1.

10.3 Transformation

Assume that a given non-linear relationship may be linearized by means of coordinate transformations. Then, initially, there will be no linearization errors which otherwise would be superimposed on the measurement errors. On the other hand, when transferring the uncertainties of the estimators of the linearized model to the estimators of the primary, non-linear model, we have to linearize as well. In a sense, which of the two approaches – linearization or transformation of a given non-linear function – turns out to be more favourable, seems to depend on the strategy aimed at.

Example

Given m measured data pairs $(\bar{x}_i, \bar{y}_i)$; $i = 1, \ldots, m$ and a non-linear relationship $\phi(x, y;\, a, b) = 0$, we shall estimate the parameters a and b. Let

$$\phi(x, y;\, a, b) = y - a x^b \,. \tag{10.109}$$

Taking logarithms yields

$$\ln y = \ln a + b \ln x \,. \tag{10.110}$$

Setting $v = \ln y$, $u = \ln x$, $\beta_1 = \ln a$, and $\beta_2 = b$ changes (10.110) into

$$\beta_1 + \beta_2 u = v \,. \tag{10.111}$$

From (10.14) and (10.89), we find the parameters and their uncertainties, say

$$\bar{\beta}_k \pm u_{\bar{\beta}_k} \,, \quad k = 1, 2 \,. \tag{10.112}$$

To estimate the uncertainty $u_{\bar{a}}$ of the parameter $\bar{a}$, we linearize

$$\bar{a} = \mathrm{e}^{\bar{\beta}_1} \tag{10.113}$$

with respect to the points $\bar{a}$ and a_0,

$$\begin{aligned} \bar{a}_l &= \bar{a} + \mathrm{e}^{\bar{\beta}_1} \left(\bar{\beta}_{1,l} - \bar{\beta}_1 \right) \,; \quad l = 1, \ldots, n \,, \\ \bar{a} &= a_0 + \mathrm{e}^{\bar{\beta}_1} \left(\bar{\beta}_1 - \bar{\beta}_{0,1} \right) \,. \end{aligned} \tag{10.114}$$

From the first expansion we obtain the uncertainty due to random errors and from the second one the uncertainty due to propagated systematic errors, so that

$$\bar{a} \pm u_{\bar{a}} \,; \quad u_{\bar{a}} = \mathrm{e}^{\bar{\beta}_1} u_{\bar{\beta}_1} \,. \tag{10.115}$$

Finally, as $b = \beta_2$, we have

$$\bar{b} \pm u_{\bar{b}} \,; \quad u_{\bar{b}} = u_{\bar{\beta}_2} \,. \tag{10.116}$$

11 Systems with Three Parameters

11.1 Planes

The adjustment of three-parametric relationships calls for coordinate triples

$$(\bar{x}_i, \bar{y}_i, \bar{z}_i)\ ; \quad i =, \ldots, m\,.$$

As usual, we assign to each of the measurands $\bar{x}_i, \bar{y}_i, \bar{z}_i$ an error equation

$$\bar{x}_i = \frac{1}{n}\sum_{l=1}^{n} x_{il} = x_{0,i} + (\bar{x}_i - \mu_{\bar{x}_i}) + f_{\bar{x}_i}\,; \quad f_{s,\bar{x}_i} \le f_{\bar{x}_i} \le f_{s,\bar{x}_i}$$

$$\bar{y}_i = \frac{1}{n}\sum_{l=1}^{n} y_{il} = y_{0,i} + (\bar{y}_i - \mu_{\bar{y}_i}) + f_{\bar{y}_i}\,; \quad f_{s,\bar{y}_i} \le f_{\bar{y}_i} \le f_{s,\bar{y}_i}$$

$$\bar{z}_i = \frac{1}{n}\sum_{l=1}^{n} z_{il} = z_{0,i} + (\bar{z}_i - \mu_{\bar{z}_i}) + f_{\bar{z}_i}\,; \quad f_{s,\bar{z}_i} \le f_{\bar{z}_i} \le f_{s,\bar{z}_i}\,.$$

Let us now consider the least squares adjustment of planes, see Fig. 11.1.

Solution Vector

Inserting $m > 4$ erroneous coordinate triples into the equation of the plane

$$z = \beta_1 + \beta_2 x + \beta_3 y \tag{11.1}$$

yields an inconsistent linear system of the kind

$$\beta_1 + \beta_2 \bar{x}_i + \beta_3 \bar{y}_i \approx \bar{z}_i\,; \quad i = 1, \ldots, m\,. \tag{11.2}$$

For convenience, we define column vectors

$$\bar{\boldsymbol{z}} = (\bar{z}_1 \quad \bar{z}_2 \quad \ldots \quad \bar{z}_3)^{\mathrm{T}}\,, \quad \boldsymbol{\beta} = (\beta_1 \quad \beta_2 \quad \beta_3)^{\mathrm{T}} \tag{11.3}$$

and a design matrix

$$\boldsymbol{A} = \begin{pmatrix} 1 & \bar{x}_1 & \bar{y}_1 \\ 1 & \bar{x}_2 & \bar{y}_2 \\ \ldots & \ldots & \ldots \\ 1 & \bar{x}_m & \bar{y}_m \end{pmatrix}$$

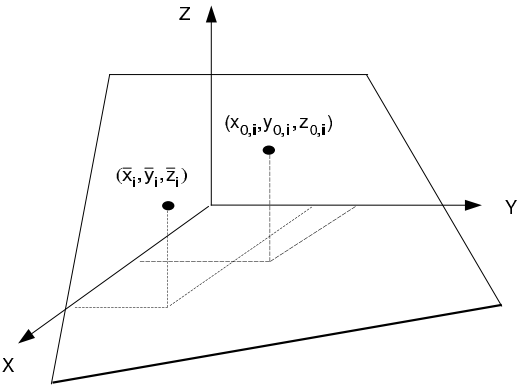


Fig. 11.1. Least squares plane, measured and true data triples

so that (11.2) turns into

$$\boldsymbol{A}\boldsymbol{\beta} \approx \bar{\boldsymbol{z}}\,. \tag{11.4}$$

The solution vector is

$$\bar{\boldsymbol{\beta}} = \boldsymbol{B}^{\mathrm{T}}\bar{\boldsymbol{z}}\,; \quad \boldsymbol{B} = \boldsymbol{A}(\boldsymbol{A}^{\mathrm{T}}\boldsymbol{A})^{-1}\,. \tag{11.5}$$

Uncertainties of the Parameters

We immediately see the difficulties incurred to estimate the measurement uncertainties and the uncertainty "bowls" which should enclose the true plane: Firstly, a (3×3) matrix has to be inverted algebraically, and, secondly, the components of the solution vector $\bar{\boldsymbol{\beta}}$ have to be linearized. However, not every user needs to bother about these procedures as there will be software packages to implement the formalism we are looking for.

Expanding the components of the solution vector (11.5) throughout a neighborhood of the point $(x_{0,1}, \ldots, x_{0,m};\ y_{0,1}, \ldots, y_{0,m};\ z_{0,1}, \ldots, z_{0,m})$ with respect to the means $\bar{x}_1, \ldots, \bar{x}_m;\ \bar{y}_1, \ldots, \bar{y}_m;\ \bar{z}_1, \ldots, \bar{z}_m$ and making use of the common approximations yields, letting $k = 1, 2, 3$,

$$\begin{aligned}
&\bar{\beta}_k\,(\bar{x}_1, \ldots, \bar{x}_m; \bar{y}_1, \ldots, \bar{y}_m; \bar{z}_1, \ldots, \bar{z}_m) \\
&= \bar{\beta}_k\,(x_{0,1}, \ldots, x_{0,m}; y_{0,1}, \ldots, y_{0,m}; z_{0,1}, \ldots, \bar{z}_{0,m}) \\
&\quad + \sum_{j=1}^{m} \frac{\partial \bar{\beta}_k}{\partial \bar{x}_j}\,(\bar{x}_j - x_{0,j}) + \sum_{j=1}^{m} \frac{\partial \bar{\beta}_k}{\partial \bar{y}_j}\,(\bar{y}_j - y_{0,j}) + \sum_{j=1}^{m} \frac{\partial \bar{\beta}_k}{\partial \bar{z}_j}\,(\bar{z}_j - z_{0,j})\ .
\end{aligned} \tag{11.6}$$

The $\beta_{0,k} = \bar{\beta}_k(x_{0,1} \ldots, x_{0,m}; y_{0,1}, \ldots, y_{0,m}; z_{0,1}, \ldots, \bar{z}_{0,m})$ designate the true values of the coefficients of the plane (11.1). The systematic errors of the estimators $\bar{\beta}_k$ are given by

$$f_{\bar\beta_k} = \sum_{j=1}^{m} \frac{\partial \bar\beta_k}{\partial \bar x_j} f_{\bar x_j} + \sum_{j=1}^{m} \frac{\partial \bar\beta_k}{\partial \bar y_j} f_{\bar y_j} + \sum_{j=1}^{m} \frac{\partial \bar\beta_k}{\partial \bar z_j} f_{\bar z_j}\,; \quad k = 1, 2, 3\,. \tag{11.7}$$

To present the empirical variance–covariance matrix of the solution vector, we expand the $\bar\beta_k$; $k = 1, 2, 3$ in

$$(\bar x_1, \ldots, \bar x_m;\, \bar y_1, \ldots, \bar y_m;\, \bar z_1, \ldots, \bar z_m)$$

with respect to the l-th individual measurements

$$x_{1l}, \ldots, x_{ml};\, y_{1l}, \ldots, y_{ml};\, z_{1l}, \ldots, z_{ml}$$

so that

$$\begin{aligned} &\bar\beta_{kl}\,(x_{1l}, \ldots, x_{ml}; y_{1l}, \ldots, y_{ml}; z_{1l}, \ldots, z_{ml}) \\ &= \bar\beta_k\,(\bar x_1, \ldots, \bar x_m; \bar y_1, \ldots, \bar y_m; \bar z_1, \ldots, \bar z_m) \\ &\quad + \sum_{j=1}^{m} \frac{\partial \bar\beta_k}{\partial \bar x_j}\,(x_{jl} - \bar x_j) + \sum_{j=1}^{m} \frac{\partial \bar\beta_k}{\partial \bar y_j}\,(y_{jl} - \bar y_j) + \sum_{j=1}^{m} \frac{\partial \bar\beta_k}{\partial \bar z_j}\,(z_{jl} - \bar z_j)\,; \end{aligned} \tag{11.8}$$

where $l = 1, \ldots, n$. The partial derivatives

$$c_{ik} = \frac{\partial \bar\beta_k}{\partial \bar x_i}\,, \quad c_{i+m,k} = \frac{\partial \bar\beta_k}{\partial \bar y_i}\,, \quad c_{i+2m,k} = \frac{\partial \bar\beta_k}{\partial \bar z_i}\,; \quad i = 1, \ldots, m \tag{11.9}$$

are given in Appendix F. To abbreviate, we introduce the notations

$$\begin{array}{lll} v_{il} = x_{il} & v_{i+m,l} = y_{il} & v_{i+2m,l} = z_{il} \\ \bar v_i = \bar x_i & \bar v_{i+m} = \bar y_i & \bar v_{i+2m} = \bar z_i \\ \mu_i = \mu_{\bar x_i} & \mu_{i+m} = \mu_{\bar y_i} & \mu_{i+2m} = \mu_{\bar z_i} \\ f_i = f_{\bar x_i} & f_{i+m} = f_{\bar y_i} & f_{i+2m} = f_{\bar z_i} \\ f_{s,i} = f_{s,\bar x_i} & f_{s,i+m} = f_{s,\bar y_i} & f_{s,i+2m} = f_{s,\bar z_i} \end{array}$$

so that (11.6) turns into

$$\bar\beta_k = \beta_{0,k} + \sum_{j=1}^{3m} c_{jk}\,(\bar v_j - \mu_j) + \sum_{j=1}^{3m} c_{jk} f_j\,; \quad k = 1, 2, 3 \tag{11.10}$$

while (11.8) yields

$$\bar\beta_{kl} - \bar\beta_k = \sum_{j=1}^{3m} c_{jk}\,(v_{jl} - \bar v_j)\,; \quad k = 1, 2, 3\,. \tag{11.11}$$

From this we find

$$
\begin{aligned}
s_{\bar{\beta}_k \bar{\beta}_{k'}} &= \frac{1}{n-1} \sum_{l=1}^{n} \left[\sum_{i=1}^{3m} c_{ik} \left(v_{il} - \bar{v}_i \right) \right] \left[\sum_{j=1}^{3m} c_{jk'} \left(v_{jl} - \bar{v}_j \right) \right] \\
&= \sum_{i,j=1}^{3m} c_{ik} c_{jk'} \left[\frac{1}{n-1} \sum_{l=1}^{n} \left(v_{il} - \bar{v}_i \right) \left(v_{jl} - \bar{v}_j \right) \right] \\
&= \sum_{i,j=1}^{3m} c_{ik} c_{jk'} s_{ij} \qquad (11.12)
\end{aligned}
$$

where the

$$
s_{ij} = \frac{1}{n-1} \sum_{l=1}^{n} \left(v_{il} - \bar{v}_i \right) \left(v_{jl} - \bar{v}_j \right) ; \quad i, j = 1, \ldots, 3m \qquad (11.13)
$$

denote the empirical variances and covariances of the input data. Assembling the s_{ij} and the c_{ik} within matrices

$$
\boldsymbol{s} = (s_{ij}) \qquad (11.14)
$$

and

$$
\boldsymbol{C}^{\mathrm{T}} = \begin{pmatrix} c_{11}\ c_{21} \cdots c_{3m,1} \\ c_{12}\ c_{22} \cdots c_{3m,2} \\ c_{13}\ c_{23} \cdots c_{3m,3} \end{pmatrix} \qquad (11.15)
$$

respectively, we may condense (11.12) to

$$
\boldsymbol{s}_{\bar{\beta}} = \boldsymbol{C}^{\mathrm{T}} \boldsymbol{s} \boldsymbol{C} \, . \qquad (11.16)
$$

Furthermore, from (11.10) we infer

$$
f_{\bar{\beta}_k} = \sum_{j=1}^{3m} c_{jk} f_j \, ; \quad k = 1, 2, 3 \, . \qquad (11.17)
$$

Finally, the uncertainties of the parameters $\bar{\beta}_k$; $k = 1, 2, 3$ of the fitted least squares plane

$$
\bar{z}(x, y) = \bar{\beta}_1 + \bar{\beta}_2 x + \bar{\beta}_3 y \qquad (11.18)
$$

are given by

$$
u_{\bar{\beta}_k} = \frac{t_P (n-1)}{\sqrt{n}} \sqrt{\sum_{i,j=1}^{3m} c_{ik} c_{jk} s_{ij}} + \sum_{j=1}^{3m} |c_{jk}| \, f_{s,j} \, ; \quad k = 1, 2, 3 \, . \qquad (11.19)
$$

Equal Systematic Errors

Let $f_{\bar{x}_i} = f_x$; $f_{\bar{y}_i} = f_y$; $f_{\bar{z}_i} = f_z$; $i = 1, \ldots, m$. Obviously, suchlike perturbations shift the least squares plane parallel to itself. Splitting up the systematic errors (11.17),

$$\begin{aligned} f_{\bar{\beta}_k} &= \sum_{j=1}^{m} c_{jk} f_{\bar{x}_j} + \sum_{j=1}^{m} c_{j+m,k} f_{\bar{y}_j} + \sum_{j=1}^{m} c_{j+2m,k} f_{\bar{z}_j} \\ &= f_x \sum_{j=1}^{m} c_{jk} + f_y \sum_{j=1}^{m} c_{j+m,k} + f_z \sum_{j=1}^{m} c_{j+2m,k}\,, \end{aligned}$$

and using

$$\begin{aligned} &\sum_{j=1}^{m} c_{j1} = -\bar{\beta}_2 \quad \sum_{j=1}^{m} c_{j+m,1} = -\bar{\beta}_3 \quad \sum_{j=1}^{m} c_{j+2m,1} = 1 \\ &\sum_{j=1}^{m} c_{j2} = 0 \qquad \sum_{j=1}^{m} c_{j+m,2} = 0 \qquad \sum_{j=1}^{m} c_{j+2m,2} = 0 \\ &\sum_{j=1}^{m} c_{j3} = 0 \qquad \sum_{j=1}^{m} c_{j+m,3} = 0 \qquad \sum_{j=1}^{m} c_{j+2m,3} = 0 \end{aligned}$$

we find

$$f_{\bar{\beta}_1} = -\bar{\beta}_2 f_x - \bar{\beta}_3 f_y + f_z\,; \quad f_{\bar{\beta}_2} = 0\,; \quad f_{\bar{\beta}_3} = 0 \tag{11.20}$$

so that

$$\begin{aligned} u_{\bar{\beta}_1} &= \frac{t_P(n-1)}{\sqrt{n}} \sqrt{\sum_{i,j=1}^{3m} c_{i1} c_{j1} s_{ij} + \left|\bar{\beta}_2\right| f_{s,x} + \left|\bar{\beta}_3\right| f_{s,y} + f_{s,z}} \\ u_{\bar{\beta}_2} &= \frac{t_P(n-1)}{\sqrt{n}} \sqrt{\sum_{i,j=1}^{3m} c_{i2} c_{j2} s_{ij}} \\ u_{\bar{\beta}_3} &= \frac{t_P(n-1)}{\sqrt{n}} \sqrt{\sum_{i,j=1}^{3m} c_{i3} c_{j3} s_{ij}}\,. \end{aligned} \tag{11.21}$$

Uncertainty "Bowl"

Inserting (11.10) into (11.18) leads to

$$\begin{aligned} \bar{z}(x,y) &= \beta_{0,1} + \beta_{0,2} x + \beta_{0,3} y \\ &\quad + \sum_{j=1}^{3m} \left(c_{j1} + c_{j2} x + c_{j3} y\right) \left(\bar{v}_j - \mu_j\right) + \sum_{j=1}^{3m} \left(c_{j1} + c_{j2} x + c_{j3} y\right) f_j\,. \end{aligned} \tag{11.22}$$

From this we read the systematic error of $\bar{z}(x, y)$,

$$f_{z(x,y)} = \sum_{j=1}^{3m} (c_{j1} + c_{j2}x + c_{j3}y)\, f_j\,, \tag{11.23}$$

and its worst case estimation

$$f_{s,z(x,y)} = \sum_{j=1}^{3m} |c_{j1} + c_{j2}x + c_{j3}y|\, f_{s,j}\,. \tag{11.24}$$

The least squares planes of the l-th individual measurements

$$\bar{z}_l = \bar{\beta}_{1l} + \bar{\beta}_{2l}x + \bar{\beta}_{3l}y\,; \quad l = 1, \ldots, n\,,$$

allow for the differences

$$\begin{aligned} \bar{z}_l - \bar{z} &= \left(\bar{\beta}_{1l} - \bar{\beta}_1\right) + \left(\bar{\beta}_{2l} - \bar{\beta}_2\right) x + \left(\bar{\beta}_{3l} - \bar{\beta}_3\right) y \\ &= \sum_{j=1}^{3m} (c_{j1} + c_{j2}x + c_{j3}y)\,(v_{jl} - \bar{v}_j)\;; \quad l = 1, \ldots, n\,. \end{aligned} \tag{11.25}$$

For any fixed x, the empirical variance turns out to be

$$s^2_{z(x,y)} = \frac{1}{n-1} \sum_{l=1}^{n} (\bar{z}_l - \bar{z})^2 = \boldsymbol{c}^{\mathrm{T}} \boldsymbol{s} \boldsymbol{c}\,, \tag{11.26}$$

where $\boldsymbol{c}$ designates the auxiliary vector

$$\boldsymbol{c} = (c_{11} + c_{12}x + c_{13}y\, c_{21} + c_{22}x + c_{23}y\, \ldots\, c_{3m,1} + c_{3m,2}x + c_{3m,3}y)^{\mathrm{T}}\,. \tag{11.27}$$

Hence the uncertainty "bowl" in which to find the true plane

$$z_0(x, y) = \beta_{0,1} + \beta_{0,2}x + \beta_{0,3}y \tag{11.28}$$

is of the form

$$\begin{aligned} &\bar{z}(x, y) \pm u_{\bar{z}(x,y)} \\ u_{\bar{z}(x,y)} &= \frac{t_P(n-1)}{\sqrt{n}} \sqrt{\boldsymbol{c}^{\mathrm{T}} \boldsymbol{s} \boldsymbol{c}} + \sum_{j=1}^{3m} |c_{j1} + c_{j2}x + c_{j3}y|\, f_{s,j}\,. \end{aligned} \tag{11.29}$$

Equal Systematic Errors

Let $f_{\bar{x}_i} = f_x$; $f_{\bar{y}_i} = f_y$; $f_{\bar{z}_i} = f_z$. As (11.23) changes into

$$f_{\bar{z}(x,y)} = -\bar{\beta}_2 f_x - \bar{\beta}_3 f_y + f_z\,,$$

we have

$$\begin{aligned} &\bar{z}(x, y) \pm u_{\bar{z}(x,y)} \\ u_{\bar{z}(x,y)} &= \frac{t_P(n-1)}{\sqrt{n}} \sqrt{\boldsymbol{c}^{\mathrm{T}} \boldsymbol{s} \boldsymbol{c}} + \left|\bar{\beta}_2\right| f_{s,x} + \left|\bar{\beta}_3\right| f_{s,y} + f_{s,z}\,. \end{aligned} \tag{11.30}$$

Finally, we may convince ourselves of $u_{\bar{z}(0,0)} = u_{\bar{\beta}_1}$.

11.2 Parabolas

Though second order curves, parabolas are linear in their parameters. In this respect, the execution of least squares fits do not pose particular problems.

Given m measured, erroneous coordinate pairs

$$(\bar{x}_1, \bar{y}_1)\ , \quad (\bar{x}_2, \bar{y}_2), \ldots, (\bar{x}_m, \bar{y}_m)\ , \tag{11.31}$$

we assume the underlying true values $(x_{0,i}, y_{0,i})$; $i = 1, \ldots, m$ to define the true parabola

$$y_0(x) = \beta_{0,1} + \beta_{0,2}x + \beta_{0,3}x^2\,. \tag{11.32}$$

Inserting the measured point into the equation $y(x) = \beta_1 + \beta_2 x + \beta_3 x^2$ leads to a linear, inconsistent system

$$\beta_1 + \beta_2\bar{x}_i + \beta_3\bar{x}_i^2 \approx \bar{y}_i\,; \quad i = 1, \ldots, m\,. \tag{11.33}$$

Let $\boldsymbol{A}$, $\boldsymbol{\beta}$ and $\bar{\boldsymbol{y}}$ denote the system matrix, the vector of the unknowns and the vector of the observations respectively,

$$\boldsymbol{A} = \begin{pmatrix} 1 & \bar{x}_1 & \bar{x}_1^2 \\ 1 & \bar{x}_2 & \bar{x}_2^2 \\ \cdots & \cdots & \cdots \\ 1 & \bar{x}_m & \bar{x}_m^2 \end{pmatrix}\ ; \quad \boldsymbol{\beta} = \begin{pmatrix} \beta_1 \\ \beta_2 \\ \beta_3 \end{pmatrix}\ ; \quad \bar{\boldsymbol{y}} = \begin{pmatrix} \bar{y}_1 \\ \bar{y}_2 \\ \cdots \\ \bar{y}_m \end{pmatrix}\ . \tag{11.34}$$

Using these definitions, we may compress (11.33) into

$$\boldsymbol{A}\boldsymbol{\beta} \approx \bar{\boldsymbol{y}}\,.$$

The least squares solution vector is

$$\bar{\boldsymbol{\beta}} = \boldsymbol{B}^{\mathrm{T}}\bar{\boldsymbol{y}}\,, \quad \boldsymbol{B} = \boldsymbol{A}\left(\boldsymbol{A}^{\mathrm{T}}\boldsymbol{A}\right)^{-1} = (b_{ik})\ . \tag{11.35}$$

11.2.1 Error-free Abscissas, Erroneous Ordinates

To begin with, we shall follow the traditional approach and assume the abscissas to be error-free. Subsequently this restriction will be suspended.

No Repeat Measurements

In the simplest case, we consider the ordinates to represent individual, erroneous measurements. Furthermore, we shall imply that each of the latter is biased by one and the same systematic error f_y so that

$$\begin{aligned} \boldsymbol{y} &= (y_1\, y_2\, \ldots\, y_m)^{\mathrm{T}} = \boldsymbol{y}_0 + (\boldsymbol{y} - \boldsymbol{\mu}) + \boldsymbol{f} \\ y_i &= y_{0,i} + (y_i - \mu_{y_i}) + f_y\,, \quad i = 1, \ldots, m\,, \end{aligned} \tag{11.36}$$

where

$$\boldsymbol{f} = f_y(\underbrace{1 \ldots 1}_{m})^{\mathrm{T}}\,; \quad -f_{s,y} \le f_y \le f_{s,y}\,.$$

The random errors $y_i - \mu_{y_i}$ are assumed to be independent and normally distributed; furthermore, they shall relate to the same parent distribution.

In (11.33), substituting true values $x_{0,i}$ for the abscissas $\bar{x}_i$, the matrix $\boldsymbol{B}$ becomes error-free. The solution vector is

$$\bar{\boldsymbol{\beta}} = \boldsymbol{B}^{\mathrm{T}}\boldsymbol{y}\,. \tag{11.37}$$

Inserting (11.36) into (11.37) yields

$$\bar{\boldsymbol{\beta}} = \boldsymbol{\beta}_0 + \boldsymbol{B}^{\mathrm{T}}(\boldsymbol{y} - \boldsymbol{\mu}) + \boldsymbol{f}_{\bar{\boldsymbol{\beta}}}\,, \quad \boldsymbol{f}_{\bar{\boldsymbol{\beta}}} = \boldsymbol{B}^{\mathrm{T}}\boldsymbol{f}\,. \tag{11.38}$$

Clearly, the components of the vector $\boldsymbol{f}_{\bar{\boldsymbol{\beta}}}$ are given by

$$f_{\bar{\beta}_1} = f_y\,, \quad f_{\bar{\beta}_2} = 0\,, \quad f_{\bar{\beta}_3} = 0\,. \tag{11.39}$$

Remarkably enough, in analogy to (10.26) and (10.27), we may prove $\boldsymbol{f}^{\mathrm{T}}\boldsymbol{f} - \boldsymbol{f}^{\mathrm{T}}\boldsymbol{P}\boldsymbol{f} = \boldsymbol{0}$ so that, following (8.11), the minimized sum of squared residuals yields an estimator

$$s_y^2 = \frac{\bar{Q}_{\text{unweighted}}}{m-3} \tag{11.40}$$

for the theoretical variance

$$\sigma_y^2 = E\left\{(Y_i - \mu_{y_i})^2\right\}\,; \quad i = 1, \ldots, m\,. \tag{11.41}$$

of the input data[1]

Uncertainties of the Components of the Solution Vector

From the components

$$\bar{\beta}_k = \sum_{i=1}^{m} b_{ik} y_i\,; \quad k = 1, 2, 3 \tag{11.42}$$

of the solution vector and its expectations

$$E\left\{\bar{\beta}_k\right\} = \mu_{\bar{\beta}_k} = \sum_{i=1}^{m} b_{ik}\mu_{y_i}\,; \quad k = 1, 2, 3\,, \tag{11.43}$$

[1] If the existence of a true parabola is doubtful, (11.40), of course, is also questionable.

we obtain the differences

$$\bar{\beta}_k - \mu_{\bar{\beta}_k} = \sum_{i=1}^{m} b_{ik\left(y_i - \mu_{y_i}\right)}\,; \quad k = 1,2,3$$

so that we can define the elements

$$\sigma_{\bar{\beta}_k \bar{\beta}_{k'}} = E\left\{\left(\bar{\beta}_k - \mu_{\bar{\beta}_k}\right)\left(\bar{\beta}_{k'} - \mu_{\bar{\beta}_{k'}}\right)\right\} = \sigma_y^2 \sum_{i=1}^{m} b_{ik} b_{ik'}\,; \quad k,k' = 1,2,3\,,$$

of the theoretical variance–covariance matrix of the solution vector $\bar{\boldsymbol{\beta}}$. According to (11.40), their empirical counterparts are given by

$$s_{\bar{\beta}_k \bar{\beta}_{k'}} = s_y^2 \sum_{i=1}^{m} b_{ik} b_{ik'}\,; \quad k,k' = 1,2,3\,. \tag{11.44}$$

Finally, the uncertainties of the estimators $\bar{\beta}_k$; $k = 1,2,3$ turn out to be

$$u_{\bar{\beta}_k} = t_P(m-3)\, s_y \sqrt{\sum_{i=1}^{m} b_{ik} b_{ik}} + f_{s,\bar{\beta}_k}\,; \quad k = 1,2,3 \tag{11.45}$$

in which, according to (11.39),

$$f_{s,\bar{\beta}_1} = f_{s,y}\,, \quad f_{s,\bar{\beta}_2} = 0\,, \quad f_{s,\bar{\beta}_3} = 0\,. \tag{11.46}$$

Uncertainty Band

Inserting the components of the solution vector (11.38),

$$\bar{\beta}_k = \beta_{0,k} + \sum_{i=1}^{m} b_{ik}\left(y_i - \mu_{y_i}\right) + f_{\bar{\beta}_k}\,; \quad k = 1,2,3\,,$$

into the fitted parabola $\bar{y}(x) = \bar{\beta}_1 + \bar{\beta}_2 x + \bar{\beta}_3 x^2$, we find

$$\bar{y}(x) = y_0(x) + \sum_{i=1}^{m} \left(b_{i1} + b_{i2} x + b_{i3} x^2\right)\left(y_i - \mu_{y_i}\right) + f_y \tag{11.47}$$

in which

$$f_y = f_{\bar{\beta}_1} \tag{11.48}$$

designates the systematic error. For any fixed x, the theoretical variance of $\bar{Y}(x)$ with respect to the expectation

$$\mu_{\bar{Y}(x)} = E\left\{\bar{Y}(x)\right\} = y_0(x) + f_y \tag{11.49}$$

yields

$$\sigma^2_{\bar{Y}(x)} = E\left\{\left(\bar{Y}(x) - \mu_{\bar{Y}(x)}\right)^2\right\} = \sigma_y^2 \sum_{i=1}^{m} \left(b_{i1} + b_{i2}x + b_{i3}x^2\right)^2 \,. \quad (11.50)$$

Hence, we expect the uncertainty band

$$\begin{aligned} &\bar{y}(x) \pm u_{\bar{y}(x)} \\ &u_{\bar{y}(x)} = t_P(m-3)s_y \sqrt{\sum_{i=1}^{m} \left(b_{i1} + b_{i2}x + b_{i3}x^2\right)^2} + f_{s,y} \end{aligned} \quad (11.51)$$

to enclose the true parabola (11.32).

Repeat Measurements

For convenience, we shall preserve the nomenclature hitherto used, i.e. we continue to denote the least squares parabola by

$$\bar{y}(x) = \bar{\beta}_1 + \bar{\beta}_2 x + \bar{\beta}_3 x^2 \,,$$

though the ordinates will now enter in the form of arithmetic means

$$\begin{aligned} &\bar{\boldsymbol{y}} = (\bar{y}_1\, \bar{y}_2\, \ldots\, \bar{y}_m)^{\mathrm{T}} \\ &\bar{y}_i = y_{0,i} + (\bar{y}_i - \mu_{\bar{y}_i}) + f_{\bar{y}_i}\,; \quad -f_{s,\bar{y}_i} \le f_{\bar{y}_i} \le f_{s,\bar{y}_i}\,. \end{aligned} \quad (11.52)$$

As usual, we assume each of the ordinates to include the same number, say n, of repeat measurements. At the same time, we dismiss the restriction that the means $\bar{y}_i$; $i = 1, \ldots, m$ are biased by one and the same systematic error.

Uncertainties of the Components of the Solution Vector

As we assume the abscissas to be error-free, so are the elements b_{ik} of the matrix $\boldsymbol{B}$. Inserting the error equations (11.52) into

$$\bar{\beta}_k = \sum_{i=1}^{m} b_{ik}\bar{y}_i\,; \quad k = 1, 2, 3 \quad (11.53)$$

yields

$$\bar{\beta}_k\,(\bar{y}_1, \ldots, \bar{y}_2) = \beta_{0,k} + \sum_{i=1}^{m} b_{ik}\,(\bar{y}_i - \mu_{\bar{y}_i}) + \sum_{i=1}^{m} b_{ik} f_{\bar{y}_i}\,. \quad (11.54)$$

Obviously, the

$$f_{\bar{\beta}_k} = \sum_{i=1}^{m} b_{ik} f_{\bar{y}_i}\,, \quad f_{s,\bar{\beta}_k} = \sum_{i=1}^{m} |b_{ik}|\, f_{s,\bar{y}_i} \quad (11.55)$$

denote the propagated systematic errors of the components $\bar{\beta}_k$; $k = 1, 2, 3$ of the solution vector. To assess the influence of random errors, we insert the means

$$\bar{y}_i = \frac{1}{n} \sum_{l=1}^{n} y_{il} \,, \quad i = 1, \ldots, m$$

into (11.53),

$$\bar{\beta}_k = \sum_{i=1}^{m} b_{ik} \left[\frac{1}{n} \sum_{l=1}^{n} y_{il} \right] = \frac{1}{n} \sum_{l=1}^{n} \left[\sum_{i=1}^{m} b_{ik} y_{il} \right] = \frac{1}{n} \sum_{l=1}^{n} \bar{\beta}_{kl} \,; \quad k = 1, 2, 3 \,. \tag{11.56}$$

Obviously, the quantities

$$\bar{\beta}_{kl} = \sum_{i=1}^{m} b_{ik} y_{il} \,; \quad k = 1, 2, 3 \,; \quad l = 1, \ldots, n \tag{11.57}$$

are the estimators of an adjustment which uses only every l-th measurement of the means $\bar{y}_i$; $i = 1, \ldots, m$. The differences

$$\bar{\beta}_{kl} - \bar{\beta}_k = \sum_{i=1}^{m} b_{ik} \left(y_{il} - \bar{y}_i \right) \,; \quad k = 1, 2, 3 \,; \quad l = 1, \ldots, n \tag{11.58}$$

lead us to the elements

$$\begin{aligned} s_{\bar{\beta}_k \bar{\beta}_{k'}} &= \frac{1}{n-1} \sum_{l=1}^{n} \left(\bar{\beta}_{kl} - \bar{\beta}_k \right) \left(\bar{\beta}_{k'l} - \bar{\beta}_{k'} \right) \\ &= \frac{1}{n-1} \sum_{l=1}^{n} \left[\sum_{i=1}^{m} b_{ik} \left(y_{il} - \bar{y}_i \right) \right] \left[\sum_{j=1}^{m} b_{jk'} \left(y_{jl} - \bar{y}_j \right) \right] \\ &= \sum_{i,j=1}^{m} b_{ik} b_{jk'} s_{ij} \,; \quad k, k' = 1, 2, 3 \end{aligned} \tag{11.59}$$

of the empirical variance–covariance matrix of the solution vector $\bar{\boldsymbol{\beta}}$. As to computer-assisted approaches, the matrix representation

$$\boldsymbol{s}_{\bar{\beta}} = \begin{pmatrix} s_{\bar{\beta}_1 \bar{\beta}_1} & s_{\bar{\beta}_1 \bar{\beta}_2} & s_{\bar{\beta}_1 \bar{\beta}_3} \\ s_{\bar{\beta}_2 \bar{\beta}_1} & s_{\bar{\beta}_2 \bar{\beta}_2} & s_{\bar{\beta}_2 \bar{\beta}_3} \\ s_{\bar{\beta}_3 \bar{\beta}_1} & s_{\bar{\beta}_3 \bar{\beta}_2} & s_{\bar{\beta}_3 \bar{\beta}_3} \end{pmatrix} = \boldsymbol{B}^{\mathrm{T}} \boldsymbol{s} \boldsymbol{B} \,; \quad s_{\bar{\beta}_k \bar{\beta}_k} \equiv s^2_{\bar{\beta}_k} \tag{11.60}$$

proves to be more convenient. The matrix

$$\boldsymbol{s} = (s_{ij}) \,, \quad s_{ij} = \frac{1}{n-1} \sum_{l=1}^{n} \left(y_{il} - \bar{y}_i \right) \left(y_{jl} - \bar{y}_j \right) \,, \quad i, j = 1, \ldots, m \tag{11.61}$$

designates the empirical variance–covariance matrix of the input data. Now we are in a position to establish Student's confidence intervals

$$\bar{\beta}_k - \frac{t_P(n-1)}{\sqrt{n}} s_{\bar{\beta}_k} \le \mu_{\bar{\beta}_k} \le \bar{\beta}_k + \frac{t_P(n-1)}{\sqrt{n}} s_{\bar{\beta}_k}\,; \quad k = 1,2,3 \quad (11.62)$$

for the expectations $E\{\bar{\beta}_k\} = \mu_{\bar{\beta}_k}$.

Finally, the overall uncertainties $u_{\bar{\beta}_k}$ of the results $\bar{\beta}_k \pm u_{\bar{\beta}_k}$; $k = 1,2,3$ turn out to be

$$u_{\bar{\beta}_k} = \frac{t_P(n-1)}{\sqrt{n}} s_{\bar{\beta}_k} + f_{s,\bar{\beta}_k} = \frac{t_P(n-1)}{\sqrt{n}} \sqrt{\sum_{i,j=1}^{m} b_{ik} b_{jk} s_{ij}} + \sum_{i=1}^{m} |b_{ik}|\, f_{s,\bar{y}_i}$$

$$k = 1,2,3\,. \quad (11.63)$$

Equal Systematic Errors

Let $f_{\bar{y}_i} = f_y$; $i = 1,\ldots,m$. The expansions given in Appendix F (where we have to substitute true abscissas $x_{0,j}$ for the means $\bar{x}_j$ quoted there) yield

$$\sum_{j=1}^{m} b_{j1} = 1\,, \quad \sum_{j=1}^{m} b_{j2} = 0\,, \quad \sum_{j=1}^{m} b_{j3} = 0\,, \quad (11.64)$$

i.e.

$$f_{\bar{\beta}_1} = f_y\,, \quad f_{\bar{\beta}_2} = 0\,, \quad f_{\bar{\beta}_3} = 0 \quad (11.65)$$

so that

$$u_{\bar{\beta}_1} = \frac{t_P(n-1)}{\sqrt{n}} \sqrt{\sum_{i,j=1}^{m} b_{i1} b_{j1} s_{ij}} + f_{s,y}$$

$$u_{\bar{\beta}_2} = \frac{t_P(n-1)}{\sqrt{n}} \sqrt{\sum_{i,j=1}^{m} b_{i2} b_{j2} s_{ij}}$$

$$u_{\bar{\beta}_3} = \frac{t_P(n-1)}{\sqrt{n}} \sqrt{\sum_{i,j=1}^{m} b_{i3} b_{j3} s_{ij}}\,. \quad (11.66)$$

Uncertainty Band

Insertion of (11.54) into the least squares parabola $\bar{y}(x) = \bar{\beta}_1 + \bar{\beta}_2 x + \bar{\beta}_3 x^2$ yields

$$\bar{y}(x) = y_0(x) + \sum_{j=1}^{m} \left(b_{j1} + b_{j2}x + b_{j3}x^2\right) \left(\bar{y}_j - \mu_{\bar{y}_j}\right)$$

$$+ \sum_{j=1}^{m} \left(b_{j1} + b_{j2}x + b_{j3}x^2\right) f_{\bar{y}_j}\,. \quad (11.67)$$

Clearly, the x-dependent systematic error is given by

$$f_{\bar{y}(x)} = \sum_{j=1}^{m} \left(b_{j1} + b_{j2}x + b_{j3}x^2\right) f_{\bar{y}_j}$$

and its worst case estimation yields

$$f_{s,\bar{y}(x)} = \sum_{j=1}^{m} \left|b_{j1} + b_{j2}x + b_{j3}x^2\right| f_{s,\bar{y}_j} \,. \tag{11.68}$$

Furthermore, from

$$\begin{aligned} \bar{y}_l(x) &= \bar{\beta}_{1,l} + \bar{\beta}_{2,l}x + \bar{\beta}_{3,l}x^2 \\ \bar{y}(x) &= \bar{\beta}_1 + \bar{\beta}_2 x + \bar{\beta}_3 x^2 \end{aligned}$$

and (11.58) we find

$$\begin{aligned} \bar{y}_l(x) - \bar{y}(x) &= \left(\bar{\beta}_{1l} - \bar{\beta}_1\right) + \left(\bar{\beta}_{2l} - \bar{\beta}_2\right) x + \left(\bar{\beta}_{3l} - \bar{\beta}_3\right) x^2 \\ &= \sum_{j=1}^{m} \left(b_{j1} + b_{j2}x + b_{j3}x^2\right) \left(y_{jl} - \bar{y}_j\right) \end{aligned} \tag{11.69}$$

so that

$$s^2_{\bar{y}(x)} = \frac{1}{n-1} \sum_{l=1}^{n} \left[y_l(x) - y(x)\right]^2 = \boldsymbol{b}^{\mathrm{T}} \boldsymbol{s} \boldsymbol{b} \,, \tag{11.70}$$

where the auxiliary vector

$$\boldsymbol{b} = \left(b_{11} + b_{12}x + b_{13}x^2 \, b_{21} + b_{22}x + b_{23}x^2 \, \ldots \, b_{m1} + b_{m2}x + b_{m3}x^2\right)^{\mathrm{T}} \tag{11.71}$$

has been introduced. The matrix $\boldsymbol{s}$ was denoted in (11.61). Ultimately, the true parabola (11.32) is expected to lie within an uncertainty band of the form

$$\begin{aligned} &\bar{y}(x) \pm u_{\bar{y}(x)} \\ u_{\bar{y}(x)} &= \frac{t_P(n-1)}{\sqrt{n}} \sqrt{\boldsymbol{b}^{\mathrm{T}} \boldsymbol{s} \boldsymbol{b}} + \sum_{j=1}^{m} \left|b_{j1} + b_{j2}x + b_{j3}x^2\right| f_{s,\bar{y}_j} \,. \end{aligned} \tag{11.72}$$

Equal Systematic Errors

Let $f_{\bar{y}_i} = f_y$; $i = 1, \ldots, m$. According to (11.64), relation (11.68) turns into $f_{s,\bar{y}(x)} = f_{s,y}$, i.e.

$$\bar{y}(x) \pm u_{\bar{y}(x)} \qquad u_{\bar{y}(x)} = \frac{t_P(n-1)}{\sqrt{n}} \sqrt{\boldsymbol{b}^{\mathrm{T}} \boldsymbol{s} \boldsymbol{b}} + f_{s,y} \,. \tag{11.73}$$

11.2.2 Erroneous Abscissas, Erroneous Ordinates

If, as is common experimental practice, both the abscissas and the ordinates are erroneous quantities, the elements b_{ik} of the matrix $\boldsymbol{B}$ as defined in (11.35) are erroneous as well. Accordingly, we linearize the estimators $\bar{\beta}_k$ twofold, namely throughout the neighborhoods of the points

$$(x_{0,1}, \ldots, x_{0,m}\,;\, y_{0,1}, \ldots, y_{0,m}) \quad \text{and} \quad (\bar{x}_1, \ldots, \bar{x}_m\,;\, \bar{y}_1, \ldots, \bar{y}_m)$$

respectively. In the former case we have

$$\begin{aligned}
&\bar{\beta}_k\,(\bar{x}_1, \ldots, \bar{x}_m;\, \bar{y}_1, \ldots, \bar{y}_m) \\
&= \bar{\beta}_k\,(x_{0,1}, \ldots, x_{0,m};\, y_{0,1}, \ldots, y_{0,m}) \\
&\quad + \sum_{j=1}^{m} \frac{\partial \bar{\beta}_k}{\partial x_{0,j}}\,(\bar{x}_j - x_{0,j}) + \sum_{j=1}^{m} \frac{\partial \bar{\beta}_k}{\partial y_{0,j}}\,(\bar{y}_j - y_{0,j}) + \cdots
\end{aligned}$$

The constants $\beta_{0,k} = \bar{\beta}_k(x_{0,1}, \ldots, x_{0,m};\, y_{0,1}, \ldots, y_{0,m})$; $k = 1, 2, 3$ denote the true values of the estimators. Furthermore, we have to relate the partial derivatives to the point $(\bar{x}_1, \ldots, \bar{x}_m;\, \bar{y}_1, \ldots, \bar{y}_m)$,

$$\frac{\partial \bar{\beta}_k}{\partial x_{0,j}} \approx \frac{\partial \bar{\beta}_k}{\partial \bar{x}_j} = c_{jk}\,, \quad \frac{\partial \bar{\beta}_k}{\partial y_{0,j}} \approx \frac{\partial \bar{\beta}_k}{\partial \bar{y}_j} = c_{j+m,k}\,; \quad j = 1, \ldots, m\,.$$

The constants $c_{jk}, c_{j+m,k}$ are quoted in Appendix F. With respect to the error equations

$$\begin{aligned}
\bar{x}_j &= x_{0,j} + \left(\bar{x}_j - \mu_{\bar{x}_j}\right) + f_{\bar{x}_j}\,; \quad -f_{s,\bar{x}_j} \le f_{\bar{x}_j} \le f_{s,\bar{x}_j} \\
\bar{y}_j &= y_{0,j} + \left(\bar{y}_j - \mu_{\bar{y}_j}\right) + f_{\bar{y}_j}\,; \quad -f_{s,\bar{y}_j} \le f_{\bar{y}_j} \le f_{s,\bar{y}_j}
\end{aligned}$$

and the second expansion which is still due, we introduce the notations

$$\begin{aligned}
&v_{jl} = x_{jl}\,; \quad v_{j+m,l} = y_{jl}\,; \quad \bar{v}_j = \bar{x}_j\,; \quad \bar{v}_{j+m} = \bar{y}_j \\
&\mu_j = \mu_{\bar{x}_j}\,; \quad \mu_{j+m} = \mu_{\bar{y}_j}\,; \quad f_j = f_{\bar{x}_j}\,; \quad f_{j+m} = f_{\bar{y}_j}\,.
\end{aligned}$$

Hence, we have

$$\bar{\beta}_k = \beta_{0,k} + \sum_{j=1}^{2m} c_{jk}\,(\bar{v}_j - \mu_j) + \sum_{j=1}^{2m} c_{jk} f_j\,; \quad k = 1, 2, 3\,. \tag{11.74}$$

From this, we infer the propagated systematic errors $f_{\bar{\beta}_k}$ of the components $\bar{\beta}_k$ as

$$f_{\bar{\beta}_k} = \sum_{j=1}^{2m} c_{jk} f_j\,; \quad k = 1, 2, 3\,.$$

The second expansion throughout a neighborhood of the point $(\bar{x}_1, \ldots, \bar{x}_m; \bar{y}_1, \ldots, \bar{y}_m)$ with respect to every l-th repeat measurement yields

$$\bar{\beta}_{kl}\,(x_{1l}, \ldots, x_{ml};\, y_{1l}, \ldots, y_{ml}) = \bar{\beta}_k\,(\bar{x}_1, \ldots, \bar{x}_m;\, \bar{y}_1, \ldots, \bar{y}_m) + \sum_{j=1}^{2m} \frac{\partial \bar{\beta}_k}{\partial \bar{x}_j}\,(x_{jl} - \bar{x}_j) + \sum_{j=1}^{2m} \frac{\partial \bar{\beta}_k}{\partial \bar{y}_j}\,(y_{jl} - \bar{y}_j) + \cdots$$

i.e.

$$\bar{\beta}_{kl} - \bar{\beta}_k = \sum_{j=1}^{2m} c_{jk}\,(v_{jl} - \bar{v}_j)\;; \quad k = 1, 2, 3\,; \quad l = 1, \ldots, n\,. \tag{11.75}$$

These differences allow the elements

$$\begin{aligned} s_{\bar{\beta}_k \bar{\beta}_{k'}} &= \frac{1}{n-1} \sum_{l=1}^{n} \left(\bar{\beta}_{kl} - \bar{\beta}_k\right) \left(\bar{\beta}_{k'l} - \bar{\beta}_{k'}\right) \\ &= \frac{1}{n-1} \sum_{l=1}^{n} \left[\sum_{i=1}^{2m} c_{ik}\,(v_{il} - \bar{v}_i)\right] \left[\sum_{j=1}^{2m} c_{jk'}\,(v_{jl} - \bar{v}_j)\right] \\ &= \sum_{i,j=1}^{2m} c_{ik} c_{jk'} s_{ij}\;; \quad k, k' = 1, 2, 3 \end{aligned} \tag{11.76}$$

of the empirical variance–covariance matrix $\bar{\boldsymbol{s}}_{\boldsymbol{\beta}}$ of the solution vector $\bar{\boldsymbol{\beta}}$ to be calculated. The s_{ij} designate the elements of the (expanded) empirical variance–covariance matrix of the input data,

$$\boldsymbol{s} = (s_{ij})\;, \quad s_{ij} = \frac{1}{n-1} \sum_{l=1}^{n} (v_{il} - \bar{v}_i)\,(v_{jl} - \bar{v}_j)\;; \quad i, j = 1, \ldots, 2m\,. \tag{11.77}$$

Finally, with the coefficients c_{ik} being comprised within the auxiliary matrix

$$\boldsymbol{C}^{\mathrm{T}} = \begin{pmatrix} c_{11}\; c_{21} \cdots c_{2m,1} \\ c_{12}\; c_{22} \cdots c_{2m,2} \\ c_{13}\; c_{23} \cdots c_{2m,3} \end{pmatrix}\,, \tag{11.78}$$

we arrive at

$$\boldsymbol{s}_{\bar{\beta}} = \begin{pmatrix} s_{\bar{\beta}_1 \bar{\beta}_1}\; s_{\bar{\beta}_1 \bar{\beta}_2}\; s_{\bar{\beta}_1 \bar{\beta}_3} \\ s_{\bar{\beta}_2 \bar{\beta}_1}\; s_{\bar{\beta}_2 \bar{\beta}_2}\; s_{\bar{\beta}_2 \bar{\beta}_3} \\ s_{\bar{\beta}_3 \bar{\beta}_1}\; s_{\bar{\beta}_3 \bar{\beta}_2}\; s_{\bar{\beta}_3 \bar{\beta}_3} \end{pmatrix} = \boldsymbol{C}^{\mathrm{T}} \boldsymbol{s} \boldsymbol{C}\,. \tag{11.79}$$

Thus, the uncertainties of the estimators $\bar{\beta}_k$; $k = 1, 2, 3$ turn out to be

$$u_{\bar{\beta}_k} = \frac{t_P (n-1)}{\sqrt{n}} \sqrt{\sum_{i,j=1}^{2m} c_{ik} c_{jk} s_{ij}} + \sum_{j=1}^{2m} |c_{jk}|\, f_{s,j}\;; \quad k = 1, 2, 3\,. \tag{11.80}$$

Equal systematic errors

Let $f_{\bar{x}_i} = f_x$, $f_{\bar{y}_i} = f_y$; $i = 1, \ldots, m$. As

$$\sum_{j=1}^{m} c_{j1} = -\bar{\beta}_2\,, \quad \sum_{j=1}^{m} c_{j+m,1} = 1\,, \quad \sum_{j=1}^{m} c_{j2} = -2\bar{\beta}_3$$
$$\sum_{j=1}^{m} c_{j+m,2} = 0\,, \quad \sum_{j=1}^{m} c_{j3} = 0\,, \quad \sum_{j=1}^{m} c_{j+m,3} = 0\,, \tag{11.81}$$

the propagated systematic errors change into

$$f_{\bar{\beta}_k} = \sum_{j=1}^{2m} c_{jk} f_j = f_x \sum_{j=1}^{m} c_{jk} + f_y \sum_{j=1}^{m} c_{j+m,k}\,; \quad k = 1, 2, 3$$

i.e.

$$f_{\bar{\beta}_1} = -\bar{\beta}_2 f_x + f_y\,; \quad f_{\bar{\beta}_2} = -2\bar{\beta}_3 f_x\,; \quad f_{\bar{\beta}_3} = 0$$

so that

$$f_{s,\bar{\beta}_1} = \left|\bar{\beta}_2\right| f_{s,x} + f_{s,y}\,; \quad f_{s,\bar{\beta}_2} = 2\left|\bar{\beta}_3\right| f_{s,x}\,; \quad f_{s,\bar{\beta}_3} = 0\,. \tag{11.82}$$

Finally, (11.80) turns into

$$u_{\bar{\beta}_1} = \frac{t_P(n-1)}{\sqrt{n}} \sqrt{\sum_{i,j=1}^{2m} c_{i1} c_{j1} s_{ij}} + \left|\bar{\beta}_2\right| f_{s,x} + f_{s,y}$$
$$u_{\bar{\beta}_2} = \frac{t_P(n-1)}{\sqrt{n}} \sqrt{\sum_{i,j=1}^{2m} c_{i2} c_{j2} s_{ij}} + 2\left|\bar{\beta}_3\right| f_{s,x}$$
$$u_{\bar{\beta}_3} = \frac{t_P(n-1)}{\sqrt{n}} \sqrt{\sum_{i,j=1}^{2m} c_{i3} c_{j3} s_{ij}}\,. \tag{11.83}$$

Uncertainty Band

Insertion of (11.74) into the least squares parabola $\bar{y}(x) = \bar{\beta}_1 + \bar{\beta}_2 x + \bar{\beta}_3 x^2$ yields

$$\bar{y}(x) = y_0(x) + \sum_{j=1}^{2m} \left(c_{j1} + c_{j2} x + c_{j3} x^2\right) (\bar{v}_j - \mu_j)$$
$$+ \sum_{j=1}^{2m} \left(c_{j1} + c_{j2} x + c_{j3} x^2\right) f_j\,. \tag{11.84}$$

Thus, the systematic error of $\bar{y}(x)$ turns out as

$$f_{\bar{y}(x)} = \sum_{j=1}^{2m} \left(c_{j1} + c_{j2}x + c_{j3}x^2\right) f_j \,. \tag{11.85}$$

We then combine

$$\bar{y}(x) = \bar{\beta}_1 + \bar{\beta}_2 x + \bar{\beta}_3 x^2$$

and

$$\bar{y}_l(x) = \bar{\beta}_{1l} + \bar{\beta}_{2l}x + \bar{\beta}_{3l}x^2 \,; \quad l = 1, \ldots, n$$

to define the n differences

$$\bar{y}_l - \bar{y} = \left(\bar{\beta}_{1l} - \bar{\beta}_1\right) + \left(\bar{\beta}_{2l} - \bar{\beta}_2\right) x + \left(\bar{\beta}_{3l} - \bar{\beta}_3\right) x^2 \,. \tag{11.86}$$

Inserting (11.75), we are in a position, for any fixed x, to quote the empirical variance of the $\bar{y}_l(x)$ with respect to $\bar{y}(x)$,

$$s^2_{\bar{y}(x)} = \frac{1}{n-1} \sum_{l=1}^{n} \left(\bar{y}_l - \bar{y}\right)^2 = \boldsymbol{c}^{\mathrm{T}} \boldsymbol{s} \boldsymbol{c} \,. \tag{11.87}$$

Here, $\boldsymbol{s}$ designates the (expanded) empirical variance–covariance matrix (11.77) of the input data and $\boldsymbol{c}$ the auxiliary vector

$$\boldsymbol{c} = \left(c_{11} + c_{12}x + c_{13}x^2 \, c_{21} + c_{22}x + c_{23}x^2 \ldots c_{2m,1} + c_{2m,2}x + c_{2m,3}x^2\right)^{\mathrm{T}} \,. \tag{11.88}$$

Hence, we expect the true parabola (11.32) to lie within the uncertainty band

$$\bar{y}(x) \pm u_{\bar{y}(x)}$$

$$u_{\bar{y}(x)} = \frac{t_P(n-1)}{\sqrt{n}} \sqrt{\boldsymbol{c}^{\mathrm{T}} \boldsymbol{s} \boldsymbol{c}} + \sum_{j=1}^{2m} \left|c_{j1} + c_{j2}x + c_{j3}x^2\right| f_{s,j} \,. \tag{11.89}$$

As may be shown, $u_{\bar{y}(0)} = u_{\bar{\beta}_1}$.

Equal Systematic Errors

Let $f_{\bar{x}_i} = f_x$, $f_{\bar{y}_i} = f_y$; $i = 1, \ldots, m$. As

$$\begin{aligned} f_{\bar{y}(x)} &= f_x \sum_{j=1}^{m} \left(c_{j1} + c_{j2}x + c_{j3}x^2\right) + f_y \sum_{j=1}^{m} \left(c_{j+m,1} + c_{j+m,2}x + c_{j+m,3}x^2\right) \\ &= -\bar{\beta}_2 f_x - 2\bar{\beta}_3 x f_x + f_y \end{aligned}$$

(11.89) changes into

$$u_{\bar{y}(x)} = \frac{t_P(n-1)}{\sqrt{n}} \sqrt{\boldsymbol{c}^{\mathrm{T}} \boldsymbol{s} \boldsymbol{c}} + \left|\bar{\beta}_2 + 2\bar{\beta}_3 x\right| f_{s,x} + f_{s,y} \,. \tag{11.90}$$

Example

Conversion of erroneous data pairs $(\bar{x}_i, \bar{y}_i)$ into data pairs $(\xi_{0,i}, \bar{\eta}_i)$ the abscissas $\xi_{0,i}$ of which are error-free while the ordinates $\bar{\eta}_i$ carry the errors of the abscissas $\bar{x}_i$ and the ordinates $\bar{y}_i$.

Let it suffice to base the conversion on, say, five neighboring data pairs $(\bar{x}_{i-2}, \bar{y}_{i-2}), \ldots, (\bar{x}_{i+2}, \bar{y}_{i+2})$. Then, every so-considered group of data defines a least squares parabola $\bar{y}(x)$ and an associated uncertainty band $u_{\bar{y}(x)}$. We simply put $\xi_{0,i} = \bar{x}_i$ and $\bar{\eta}_i = \bar{y}(\xi_{0,i})$. We may then define $\bar{y}_l(\xi_{0,i})$; $l = 1, \ldots, n$, so that

$$\bar{\eta}_i = \bar{y}\,(\xi_{0,i}) = \frac{1}{n} \sum_{l=1}^{n} \bar{y}_l\,(\xi_{0,i})\ .$$

The uncertainty $u_{\bar{y}(\xi_{0,i})}$ has been quoted in (11.89).

11.3 Piecewise Smooth Approximation

Suppose we want to approximate an empirical function, defined through a sequence of data pairs $(\bar{x}_i, \bar{y}_i)$; $i = 1, \ldots$ by a string of consecutive parabolas the junctions of which shall be continuous and differentiable, Fig. 11.2. For simplicity, we shall restrict ourselves to two consecutive parabolas so that there is but one junction. We shall presume that there are sufficiently many measuring points within the regions of approximation, so that it is possible to substitute points $\xi_{0,i}, \bar{\eta}_i$ for the measuring points $(\bar{x}_i, \bar{y}_i)$, the abscissas $\xi_{0,i}$ of which may be considered error-free while the ordinates $\bar{\eta}_i$ include the errors of the abscissas $\bar{x}_i$ and the ordinates $\bar{y}_i$. This idea has been outlined at the end of the preceding section. Let us assume that the transformations have already been done and that, for convenience, our common notation $(x_{0,i}, \bar{y}_i)$; $i = 1, 2, \ldots$ has been reintroduced.

Solution Vector

Let ξ_2 designate the junction of parabolas I and II. We then have

$$\begin{aligned} y_{\mathrm{I}}(x) &= \beta_1 + \beta_2 x + \beta_3 x^2\,; \quad \xi_1 \le x < \xi_2 \\ y_{\mathrm{II}}(x) &= \beta_4 + \beta_5 x + \beta_6 x^2\,; \quad \xi_2 \le x < \xi_3\,. \end{aligned} \tag{11.91}$$

Obviously, the parabolas have to satisfy the conditions

$$y_{\mathrm{I}}\,(\xi_2) = y_{\mathrm{II}}\,(\xi_2)\ ; \quad y'_{\mathrm{I}}\,(\xi_2) = y'_{\mathrm{II}}\,(\xi_2)\ . \tag{11.92}$$

Defining the column vector

$$\boldsymbol{\beta} = (\beta_1\,\beta_2\,\beta_3\,\beta_4\,\beta_5\,\beta_6)^{\mathrm{T}}\ , \tag{11.93}$$

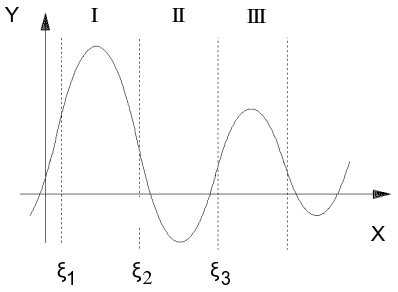


Fig. 11.2. Consecutive parabolas with continuous and differentiable junctions for piecewise smooth approximation of an empirical function

according to (7.15), we require

$$\boldsymbol{H}\boldsymbol{\beta} = \mathbf{0}\,, \tag{11.94}$$

where

$$\boldsymbol{H} = \begin{pmatrix} 1 & \xi_2 & \xi_2^2 & -1 & -\xi_2 & -\xi_2^2 \\ 0 & 1 & 2\xi_2 & 0 & -1 & -2\xi_2 \end{pmatrix}. \tag{11.95}$$

To stress, the β_k; $k = 1, \ldots, 6$ do not define a common polynomial; nevertheless we shall adjust them in one single step. The parabolas defined in (11.91) give rise to two inconsistent systems

$$\begin{aligned} &\beta_1 + \beta_2 x_{0,i} + \beta_3 x_{0,i}^2 \approx \bar{y}_i\,; \quad i = 1, \ldots, m_1 \\ &\beta_4 + \beta_5 x_{0,i} + \beta_6 x_{0,i}^2 \approx \bar{y}_i\,; \quad i = m_1 + 1, \ldots, m_1 + m_2 = m\,. \end{aligned} \tag{11.96}$$

Let us assign the means

$$\bar{y}_i = \frac{1}{n} \sum_{l=1}^{n} y_{il}\,; \quad i = 1, \ldots, m \tag{11.97}$$

to a column vector

$$\bar{\boldsymbol{y}} = (\bar{y}_1\, \bar{y}_2\, \ldots\, \bar{y}_m)^{\mathrm{T}} \tag{11.98}$$

and the coefficients $1, x_{0,i}, x_{0,i}^2$ to a system matrix of the form

$$\boldsymbol{A} = \left(\begin{array}{ccc|ccc} 1 & x_{0,1} & x_{0,1}^2 & 0 & 0 & 0 \\ \ldots & \ldots & \ldots & \ldots & \ldots & \ldots \\ 1 & x_{0,m_1} & x_{0,m_1}^2 & 0 & 0 & 0 \\ \hline 0 & 0 & 0 & 1 & x_{0,m_1+1} & x_{0,m_1+1}^2 \\ \ldots & \ldots & \ldots & \ldots & \ldots & \ldots \\ 0 & 0 & 0 & 1 & x_{0,m} & x_{0,m}^2 \end{array}\right). \tag{11.99}$$

Then, (11.96) turns into

$$\boldsymbol{A}\boldsymbol{\beta} \approx \bar{\boldsymbol{y}}\,. \tag{11.99}$$

The solution vector follows from (7.16),

$$\begin{aligned}\bar{\boldsymbol{\beta}} = \Big[&\left(\boldsymbol{A}^{\mathrm{T}}\boldsymbol{A}\right)^{-1}\boldsymbol{A}^{\mathrm{T}}\left(\boldsymbol{A}^{\mathrm{T}}\boldsymbol{A}\right)^{-1}\boldsymbol{H}^{\mathrm{T}} \\ &\times\left[\boldsymbol{H}\left(\boldsymbol{A}^{\mathrm{T}}\boldsymbol{A}\right)^{-1}\boldsymbol{H}^{\mathrm{T}}\right]^{-1}\boldsymbol{H}\left(\boldsymbol{A}^{\mathrm{T}}\boldsymbol{A}\right)^{-1}\boldsymbol{A}^{\mathrm{T}}\Big]\,\bar{\boldsymbol{y}}\,.\end{aligned} \tag{11.100}$$

To abbreviate, we assign a matrix $\boldsymbol{D}^{\mathrm{T}}$ to the outer square brackets, so that

$$\bar{\boldsymbol{\beta}} = \boldsymbol{D}^{\mathrm{T}}\bar{\boldsymbol{y}}\,; \quad \boldsymbol{D} = (d_{ik})\ , \tag{11.101}$$

$$\begin{pmatrix} \bar{\beta}_1 \\ \bar{\beta}_2 \\ \bar{\beta}_3 \\ -- \\ \bar{\beta}_4 \\ \bar{\beta}_5 \\ \bar{\beta}_6 \end{pmatrix} = \begin{pmatrix} d_{11} & d_{21} & \dots & d_{m1} \\ d_{12} & d_{22} & \dots & d_{m2} \\ d_{13} & d_{23} & \dots & d_{m3} \\ -- & -- & -- & -- \\ d_{14} & d_{24} & \dots & d_{m4} \\ d_{15} & d_{25} & \dots & d_{m5} \\ d_{16} & d_{26} & \dots & d_{m6} \end{pmatrix} \begin{pmatrix} \bar{y}_1 \\ \bar{y}_2 \\ \dots \\ \bar{y}_m \end{pmatrix}$$

in components,

$$\bar{\beta}_k = \sum_{i=1}^{m} d_{ik}\bar{y}_i\,; \quad k = 1, \dots, 6\,. \tag{11.102}$$

Uncertainty Band of a String of Parabolas

For simplicity, we confine ourselves to the uncertainty band of the fitted parabola

$$\bar{y}_I(x) = \bar{\beta}_1 + \bar{\beta}_2 x + \bar{\beta}_3 x^2\,. \tag{11.103}$$

Obviously, this formally agrees with (11.72),

$$\begin{aligned}&\bar{y}_I(x) \pm u_{\bar{y}_I(x)} \\ u_{\bar{y}_I(x)} = &\frac{t_P(n-1)}{\sqrt{n}}\sqrt{\boldsymbol{d}_{\mathrm{I}}^{\mathrm{T}}\boldsymbol{s}\boldsymbol{d}_{\mathrm{I}}} + \sum_{i=1}^{m}\left|d_{i1} + d_{i2}x + d_{i3}x^2\right| f_{s,\bar{y}_i}\,,\end{aligned} \tag{11.104}$$

where the auxiliary vector

$$\boldsymbol{d}_{\mathrm{I}} = \left(d_{11} + d_{12}x + d_{13}x^2\; d_{21} + d_{22}x + d_{23}x^2 \dots d_{m1} + d_{m2}x + d_{m3}x^2\right)^{\mathrm{T}} \tag{11.105}$$

corresponds to (11.71) and the matrix $\boldsymbol{s}$ to (11.61). With respect to the fitted parabola $\bar{\boldsymbol{y}}_{\mathrm{II}}(x)$ we have just two modifications to make: In the uncertainty component due to random errors we have to substitute an auxiliary vector

$$\boldsymbol{d}_{\mathrm{II}} = \left(d_{14} + d_{15}x + d_{16}x^2\, d_{24} + d_{25}x + d_{26}x^2 \ldots d_{m4} + d_{m5}x + d_{m6}x^2\right)^{\mathrm{T}} \tag{11.106}$$

for $\boldsymbol{d}_{\mathrm{I}}$, and in the uncertainty component due to systematic errors the matrix elements d_{i4}, d_{i5}, d_{i6} for the elements d_{i1}, d_{i2}, d_{i3}. Obviously, any error combination yields a continuous and differentiable string of parabolas.

The procedure may be generalized to more than two regions of approximation, e.g. to three regions, implying junctions ξ_1 and ξ_2, then the matrix $\boldsymbol{H}$ takes the form

$$\boldsymbol{H} = \left(\begin{array}{ccc|ccc|ccc} 1 & \xi_1 & \xi_1^2 & -1 & -\xi_1 & -\xi_1^2 & 0 & 0 & 0 \\ 0 & 1 & 2\xi_1 & 0 & -1 & -2\xi_1 & 0 & 0 & 0 \\ -- & -- & -- & -- & -- & -- & -- & -- & -- \\ 0 & 0 & 0 & 1 & \xi_2 & \xi_2^2 & -1 & -\xi_2 & -\xi_2^2 \\ 0 & 0 & 0 & 0 & 1 & 2\xi_2 & 0 & -1 & -2\xi_2 \end{array}\right) . \tag{11.107}$$

11.4 Circles

In contrast to polynomials, the equation of a circle is non-linear in the parameters to be adjusted. Consequently, we first have to linearize. This can be done either by truncating a series expansion or through a transformation, namely a stereographic projection[2]. We here will content ourselves with series truncation.

Linearization

As has been discussed in Sect. 10.2, we expand the circle's equation

$$\phi(r, x_M, y_M; x, y) = r^2 - (x - x_M)^2 - (y - y_M)^2 = 0 \tag{11.108}$$

throughout a neighborhood of some starting values r^*, x_M^*, y_M^*,

$$\begin{aligned} &\phi(r, x_M, y_M; x, y) = \phi\left(r^*, x_M^*, y_M^*; x, y\right) \\ &+ \frac{\partial\phi}{\partial r^*}\left(r - r^*\right) + \frac{\partial\phi}{\partial x_M^*}\left(x_M - x_M^*\right) + \frac{\partial\phi}{\partial y_M^*}\left(y_M - y_M^*\right) + \cdots = 0\,. \end{aligned} \tag{11.109}$$

As

$$\frac{\partial\phi}{\partial r^*} = 2r^*\,, \quad \frac{\partial\phi}{\partial x_M^*} = 2(x - x_M^*)\,, \quad \frac{\partial\phi}{\partial y_M^*} = 2(y - y_M^*)$$

[2] E.g. Knopp, K., *Elemente der Funktionentheorie*, Sammlung Göschen, vol. 1109, Walter de Gruyter, Berlin 1963

we find, truncating non-linear terms,

$$r^{*\,2} - (x - x_M^*)^2 - (y - y_M^*)^2 \tag{11.110}$$
$$+\, 2r^*\,(r - r^*) + 2\,(x - x_M^*)\,(x_M - x_M^*) + 2\,(y - y_M^*)\,(y_M - y_M^*) \approx 0\,.$$

Introducing the abbreviations

$$\begin{aligned} \beta_1 &= r - r^*\,, \quad \beta_2 = x_M - x_M^*\,, \quad \beta_3 = y_M - y_M^* \\ u(x) &= \frac{x - x_M^*}{r^*}\,, \quad v(y) = \frac{y - y_M^*}{r^*} \\ w(x,y) &= \frac{1}{2r^*}\left[(x - x_M^*)^2 + (y - y_M^*)^2 - r^{*\,2}\right] \end{aligned} \tag{11.111}$$

the expansion (11.110) turns into

$$\beta_1 + u(x)\beta_2 + v(y)\beta_3 \approx w(x,y)\,. \tag{11.112}$$

Obviously, in a formal sense, (11.112) is the equation of a plane. In order to reduce the linearization errors, we cyclically repeat the adjustment, each time replacing the "old" starting values with improved "new" ones.

Suppose there are $m \geq 4$ measured data pairs $(\bar{x}_i, \bar{y}_i)$; $i = 1, \ldots, m$, lying in the vicinity of the circumference of the circle and having the structure

$$\begin{aligned} \bar{x}_i &= \frac{1}{n}\sum_{l=1}^{n} x_{il} = x_{0,i} + (\bar{x}_i - \mu_{\bar{x}_i}) + f_{\bar{x}_i}\,, \\ \bar{y}_i &= \frac{1}{n}\sum_{l=1}^{n} y_{il} = y_{0,i} + (\bar{y}_i - \mu_{\bar{y}_i}) + f_{\bar{y}_i}\,. \end{aligned}$$

Inserting the latter into (11.112)) produces the linear, inconsistent system

$$\beta_1 + u\,(\bar{x}_i)\,\beta_2 + v\,(\bar{y}_i)\,\beta_3 \approx w\,(\bar{x}_i, \bar{y}_i)\;; \quad i = 1, \ldots, m\,. \tag{11.113}$$

The system matrix $\boldsymbol{A}$, the column vector $\boldsymbol{\beta}$ of the unknowns and the column vector $\bar{\boldsymbol{w}}$ of the right-hand sides

$$\boldsymbol{A} = \begin{pmatrix} 1 & \bar{u}_1 & \bar{v}_1 \\ 1 & \bar{u}_2 & \bar{v}_2 \\ \ldots & \ldots & \ldots \\ 1 & \bar{u}_m & \bar{v}_m \end{pmatrix}\;; \quad \boldsymbol{\beta} = \begin{pmatrix} \beta_1 \\ \beta_2 \\ \beta_3 \end{pmatrix}\;; \quad \bar{\boldsymbol{w}} = \begin{pmatrix} \bar{w}_1 \\ \bar{w}_2 \\ \ldots \\ \bar{w}_m \end{pmatrix}\,,$$

turn (11.113) into

$$\boldsymbol{A}\boldsymbol{\beta} \approx \bar{\boldsymbol{w}}\,. \tag{11.114}$$

Iteration of the Solution Vector

The least squares solution vector is

$$\bar{\boldsymbol{\beta}} = \boldsymbol{B}^{\mathrm{T}} \bar{\boldsymbol{w}}\,, \quad \boldsymbol{B} = \boldsymbol{A}\left(\boldsymbol{A}^{\mathrm{T}}\boldsymbol{A}\right)^{-1}\,. \tag{11.115}$$

Its components $\bar{\beta}_1, \bar{\beta}_2, \bar{\beta}_3$ define the parameters of the circle,

$$\bar{r} = \bar{\beta}_1 + r^*\,, \quad \bar{x}_M = \bar{\beta}_2 + x_M^*\,, \quad \bar{y}_M = \bar{\beta}_3 + y_M^*\,. \tag{11.116}$$

Interpreting the results $\bar{r}, \bar{x}_M, \bar{y}_M$ as new, improved starting values $r^* x_M^*, y_M^*$, we are in a position to cyclically repeat the adjustment. As has been discussed in Sect. 10.2, we expect the estimators to tend to zero,

$$\beta_1 \to 0,\ \beta_2 \to 0,\ \beta_3 \to 0\,.$$

This will, however, be the case only as far as allowed by the measurement errors (and, if so, by the accuracy of the machine). In

$$\bar{\beta}_k = \sum_{j=1}^{m} b_{jk} \bar{w}_j\,; \quad k = 1,2,3 \tag{11.117}$$

the coefficients b_{jk} as well as the quantities $\bar{w}_j$ prove to be erroneous.

Uncertainties of the Parameters of the Circle

In order to estimate the uncertainties, we carry out series expansions throughout the neighborhoods of the points

$$(x_{0,1}, \ldots, x_{0,m}\,;\, y_{0,1}, \ldots, y_{0,m}) \quad \text{and} \quad (\bar{x}_1, \ldots, \bar{x}_m\,;\, \bar{y}_1, \ldots, \bar{y}_m)\,.$$

The former leads us to the propagated systematic errors and the latter to the empirical variance–covariance matrix of the components $\bar{\beta}_k$; $k = 1,2,3$ of the solution vector respectively. The expansion with respect to the true values yields

$$\begin{aligned} \bar{\beta}_k\,(\bar{x}_1, \ldots, \bar{y}_m) &= \bar{\beta}_k\,(x_{0,1}, \ldots, y_{0,m}) \\ &+ \sum_{j=1}^{m} \frac{\partial \bar{\beta}_k}{\partial x_{0,j}}\,(\bar{x}_j - x_{0,j}) + \sum_{j=1}^{m} \frac{\partial \bar{\beta}_k}{\partial y_{0,j}}\,(\bar{y}_j - y_{0,j}) + \cdots\,; \quad k = 1,2,3\,. \end{aligned} \tag{11.118}$$

As usual, we linearize the expansion and approximate the partial derivatives according to

$$\frac{\partial \bar{\beta}_k}{\partial \bar{x}_{0,j}} \approx \frac{\partial \bar{\beta}_k}{\partial \bar{x}_j} = c_{jk}\,, \quad \frac{\partial \bar{\beta}_k}{\partial \bar{y}_{0,j}} \approx \frac{\partial \bar{\beta}_k}{\partial \bar{y}_j} = c_{j+m,k}\,; \quad k = 1,2,3\,, \quad j = 1, \ldots, m\,.$$

The coefficients c_{jk} and $c_{j+m,k}$ are given in Appendix F. Furthermore, we introduce

$$f_j = f_{\bar{x}_j}\,, \quad f_{j+m} = f_{\bar{y}_j}\,; \quad j = 1, \ldots, m\,.$$

Then, according to (11.118), the propagated systematic errors of the $\bar{\beta}_k$; $k = 1, 2, 3$ turn out as

$$f_{\bar{\beta}_k} = \sum_{j=1}^{2m} c_{jk} f_j\,, \quad f_{s,\,\bar{\beta}_k} = \sum_{j=1}^{2m} |c_{jk}|\, f_{s,j}\,; \quad k = 1, 2, 3\,. \tag{11.119}$$

The variances and covariances follow from the second expansion

$$\begin{aligned} \bar{\beta}_{kl}\,(x_{1l}, \ldots, y_{ml}) &= \bar{\beta}_k\,(\bar{x}_1, \ldots, \bar{y}_m) \\ &+ \sum_{j=1}^{m} \frac{\partial \bar{\beta}_k}{\partial \bar{x}_j}\,(x_{jl} - \bar{x}_j) + \sum_{j=1}^{m} \frac{\partial \bar{\beta}_k}{\partial \bar{y}_j}\,(y_{jl} - \bar{y}_j) + \cdots\,. \end{aligned} \tag{11.120}$$

We define

$$\begin{aligned} v_{jl} &= x_{jl}\,, \quad v_{j+m,l} = y_{jl}\,, \quad \bar{v}_j = \bar{x}_j\,, \quad \bar{v}_{j+m} = \bar{y}_j \\ \mu_j &= \mu_{\bar{x}_j}\,, \quad \mu_{j+m} = \mu_{\bar{y}_j}\,; \quad j = 1, \ldots, m \end{aligned}$$

so that

$$\bar{\beta}_{kl} - \bar{\beta}_k = \sum_{j=1}^{2m} c_{jk}\,(v_{jl} - \bar{v}_j)\,, \quad k = 1, 2, 3\,, \quad l = 1, \ldots, n\,. \tag{11.121}$$

From this we obtain

$$\begin{aligned} s_{\bar{\beta}_k \bar{\beta}_{k'}} &= \frac{1}{n-1} \sum_{l=1}^{n} \left[\sum_{i=1}^{2m} c_{ik}\,(v_{il} - \bar{v}_i)\right] \left[\sum_{j=1}^{2m} c_{jk'}\,(v_{jl} - \bar{v}_j)\right] \\ &= \sum_{i,j=1}^{2m} c_{ik} c_{jk} s_{ij}\,; \quad k, k' = 1, 2, 3\,. \end{aligned} \tag{11.122}$$

Assigning the coefficients c_{jk} to the $(2m \times 3)$ auxiliary matrix

$$\boldsymbol{C}^{\mathrm{T}} = \begin{pmatrix} c_{11}\; c_{21}\; \ldots\; c_{2m,1} \\ c_{12}\; c_{22}\; \ldots\; c_{2m,2} \\ c_{13}\; c_{23}\; \ldots\; c_{2m,3} \end{pmatrix} \tag{11.123}$$

the empirical variance–covariance matrix of the solution vector $\bar{\boldsymbol{\beta}}$ takes the form

$$\boldsymbol{s}_{\bar{\boldsymbol{\beta}}} = \begin{pmatrix} s_{\bar{\beta}_1 \bar{\beta}_1}\; s_{\bar{\beta}_1 \bar{\beta}_2}\; s_{\bar{\beta}_1 \bar{\beta}_3} \\ s_{\bar{\beta}_2 \bar{\beta}_1}\; s_{\bar{\beta}_2 \bar{\beta}_2}\; s_{\bar{\beta}_2 \bar{\beta}_3} \\ s_{\bar{\beta}_3 \bar{\beta}_1}\; s_{\bar{\beta}_3 \bar{\beta}_2}\; s_{\bar{\beta}_3 \bar{\beta}_3} \end{pmatrix} = \boldsymbol{C}^{\mathrm{T}} \boldsymbol{s} \boldsymbol{C}\,; \quad s_{\bar{\beta}_k \bar{\beta}_k} \equiv s^2_{\bar{\beta}_k}\,. \tag{11.124}$$

Here

$$\boldsymbol{s} = (s_{ij}) \; ; \quad i,j = 1,\ldots,2m \, , \quad s_{ij} = \frac{1}{n-1} \sum_{l=1}^{n} (v_{il} - \bar{v}_i)\,(v_{jl} - \bar{v}_j) \tag{11.125}$$

denotes the empirical variance–covariance matrix of the input data. After all, the primary results of the adjustment are given by

$$\bar{\beta}_k \pm u_{\bar{\beta}_k} \tag{11.126}$$

$$u_{\bar{\beta}_k} = \frac{t_P(n-1)}{\sqrt{n}} \sqrt{\sum_{i,j=1}^{2m} c_{ik} c_{jk} s_{ij}} + \sum_{j=1}^{2m} |c_{jk}|\, f_{s,j} \; ; \quad k = 1,2,3 \, .$$

The parameters of circle follow from

$$\bar{r} = \bar{\beta}_1 + r^* \, , \quad \bar{x}_M = \bar{\beta}_2 + \bar{x}^*_M \, , \quad \bar{y}_M = \bar{\beta}_3 + \bar{y}^*_M \, .$$

The uncertainties of the latter are, of course, identical with those of the $\bar{\beta}_k$; $k = 1,2,3$.

Equal Systematic Errors

Let $f_{\bar{x}_i} = f_x$; $f_{\bar{y}_i} = f_y$; $i = 1,\ldots,m$. As (11.119) changes into

$$f_{\bar{\beta}_k} = f_x \sum_{j=1}^{m} c_{jk} + f_y \sum_{j=1}^{m} c_{j+m,k} \; ; \quad k = 1,2,3 \, , \tag{11.127}$$

according to Appendix F we find

$$\sum_{j=1}^{m} c_{j1} = -\frac{\bar{\beta}_2}{r^*} \; ; \quad \sum_{j=1}^{m} c_{j+m,1} = -\frac{\bar{\beta}_3}{r^*} \; ; \quad \sum_{j=1}^{m} c_{j2} = 1$$

$$\sum_{j=1}^{m} c_{j+m,2} = 0 \; ; \quad \sum_{j=1}^{m} c_{j,3} = 0 \; ; \quad \sum_{j=1}^{m} c_{j+m,3} = 1 \, . \tag{11.128}$$

The propagated systematic errors become

$$f_{\bar{\beta}_1} = -\frac{1}{r^*} \left(\bar{\beta}_2 f_x + \bar{\beta}_3 f_y \right) \approx 0 \; ; \quad f_{\bar{\beta}_2} = f_x \, , \quad f_{\bar{\beta}_3} = f_y \tag{11.129}$$

so that[3]

$$u_{\bar{\beta}_1} = \frac{t_P(n-1)}{\sqrt{n}} s_{\bar{\beta}_1} \, , \quad u_{\bar{\beta}_2} = \frac{t_P(n-1)}{\sqrt{n}} s_{\bar{\beta}_2} + f_{s,x}$$

$$u_{\bar{\beta}_3} = \frac{t_P(n-1)}{\sqrt{n}} s_{\bar{\beta}_3} + f_{s,y} \, . \tag{11.130}$$

[3] On finishing the iteration, the absolute values of the estimators $\bar{\beta}_2$ and $\bar{\beta}_3$ will be very small so that $f_{\bar{\beta}_1}$ will be close to zero – the radius remains insensitive to shifts of the center of the circle.

Uncertainty Regions

From (11.111) we conclude

$$\bar{\beta}_1 = \bar{r} - r^* \,; \quad \mu_{\bar{\beta}_1} = E\{\bar{\beta}_1\} = E\{\bar{r}\} - r^* = \mu_{\bar{r}} - r^* \,,$$

i.e.

$$\bar{\beta}_1 - \mu_{\bar{\beta}_1} = \bar{r} - \mu_{\bar{r}} \,,$$

and, similarly,

$$\bar{\beta}_2 - \mu_{\bar{\beta}_2} = \bar{x}_M - \mu_{\bar{x}_M} \,; \quad \bar{\beta}_3 - \mu_{\bar{\beta}_3} = \bar{y}_M - \mu_{\bar{y}_M}$$

so that

$$\bar{\boldsymbol{\beta}} - \boldsymbol{\mu}_{\bar{\beta}} = \left(\bar{r} - \mu_{\bar{r}}\, \bar{x}_M - \mu_{\bar{x}_M}\, \bar{y}_M - \mu_{\bar{y}_M}\right)^{\mathrm{T}} \,. \tag{11.131}$$

Referring to Hotelling's ellipsoid (9.64)

$$t_P^2(r,n) = n\left(\bar{\boldsymbol{\beta}} - \boldsymbol{\mu}_{\bar{\boldsymbol{\beta}}}\right)^{\mathrm{T}} \left(\boldsymbol{C}^{\mathrm{T}} \boldsymbol{s} \boldsymbol{C}\right)^{-1} \left(\bar{\boldsymbol{\beta}} - \boldsymbol{\mu}_{\bar{\boldsymbol{\beta}}}\right) \tag{11.132}$$

we may replace $\bar{\boldsymbol{\beta}} - \boldsymbol{\mu}_{\bar{\beta}}$ by a vector of the kind

$$\left(\boldsymbol{\beta} - \bar{\boldsymbol{\beta}}\right) = \left(r - \bar{r}\, x - \bar{x}_M\, y - \bar{y}_M\right)^{\mathrm{T}} \tag{11.133}$$

so that (11.132) takes the form of a confidence ellipsoid

$$t_P^2(r,n) = n\left(\boldsymbol{\beta} - \bar{\boldsymbol{\beta}}\right)^{\mathrm{T}} \left(\boldsymbol{C}^{\mathrm{T}} \boldsymbol{s} \boldsymbol{C}\right)^{-1} \left(\boldsymbol{\beta} - \bar{\boldsymbol{\beta}}\right) \tag{11.134}$$

which we depict in a rectangular r, x_M, y_M coordinate system. Combining (11.134) with the pertaining security polyhedron produces the **EPC** hull, the procedure turning out to be more simple in case we restrict ourselves to the degeneration presented in (11.129).

There are two uncertainty regions to be constructed: a very small inner circular region, enclosing the admissible centers and a much larger, outer annular region, marking off the set of allowable circles. The inner region is given by the projection of the **EPC** hull onto the x_M, y_M-plane.

To find the outer region, we proceed numerically. To this end, we put a bunch of rays through the point $\bar{x}_M, \bar{y}_M$ covering the angular range $0, \ldots, 2\pi$ uniformly and densely enough.

Let us intersect the **EPC** hull with a plane perpendicular to the r-axis and consider the orthogonal projection of the intersection onto the x_M, y_M-plane. Obviously, each point of the so-projected line represents an admissible center (centers lying in the interior are of no interest). Each of the centers has the same radius, namely that which is given by the height of the intersecting plane. Repeating the procedure with a sufficiently closely spaced system

of intersecting planes produces the set of all admissible centers and circles. We then consider the intersections of the circles with the rays of the bunch. Sorting the intersections on a given ray according to their distances from the point $\bar{x}_M, \bar{y}_M$, the intersection with the largest distance obviously establishes a point of the outer boundary of the ring-shaped uncertainty region in question while the intersection with the smallest distance marks a point of the inner boundary of that region.

12 Special Metrology Systems

12.1 Dissemination of Units

Two basic procedures are available for disseminating units: the linking of so-called working standards to primary standards and the intercomparison of standards (of any kind) through what is called key comparisons.

12.1.1 Realization of Working Standards

The primary standards of the SI units are the starting points for the realization of day-to-day employed working standards. By nature, the accuracy such standards should have, depends on their field of application. This aspect has led to a hierarchy of standards of decreasing accuracies. Being established, we shall denote the pertaining "ranks" by H_k; $k = 1, 2, \ldots$ and use growing k to express decreasing accuracy.

Suppose the comparator operates by means of an equation of the kind

$$\beta_k = \beta_{k-1} + x\,; \quad k = 1, 2, \ldots\,. \tag{12.1}$$

Here, β_k designates the standard of rank H_k, which is to be calibrated, β_{k-1} the standard of rank H_{k-1}, which accomplishes the link-up, and, finally, x the difference shown in the comparator display. Normally, any link-up implies a loss of accuracy. Let us assume $l = 1, \ldots, n$ repeat measurements

$$x_l = x_0 + (x_l - \mu_x) + f_x\,; \quad l = 1, \ldots, n\,, \tag{12.2}$$

where x_0 designates the true value of the displayed difference x_l, $\varepsilon_l = x_l - \mu_x$ a random and f_x a systematic error. The n repeat measurements define an arithmetic mean and an empirical variance,

$$\bar{x} = \frac{1}{n}\sum_{l=1}^{n} x_l\,; \quad s_{\bar{x}}^2 = \frac{1}{n-1}\sum_{l=1}^{n}(x_l - \bar{x})^2\,. \tag{12.3}$$

Let the systematic error f_x be contained within an interval

$$-f_{s,x} \le f_x \le f_{s,x}\,. \tag{12.4}$$

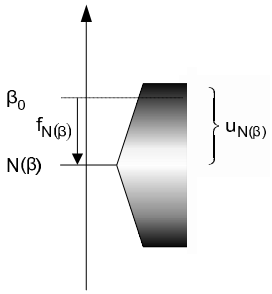


Fig. 12.1. Primary standard: nominal value $N(\beta)$ and true value β_0

Then, the interval

$$\bar{x} - u_{\bar{x}} \leq x_0 \leq \bar{x} + u_{\bar{x}}\,; \quad u_{\bar{x}} = \frac{t_P(n-1)}{\sqrt{n}} s_{\bar{x}} + f_{s,x} \tag{12.5}$$

should localize the true value x_0 of the differences x_l; $l = 1, \ldots, n$.

Let $N(\beta)$ denote the nominal value of a given primary standard, e.g. $N(\beta) = 1\,\mathrm{kg}$ (exact) and β_0 its actual, physically true value, which, of course, is unknown. Let the nominal value and the true value differ by an unknown systematic error $f_{N(\beta)}$, which we assume to be confined to the interval $-u_{N(\beta)}, \ldots, u_{N(\beta)}$. We then have, Fig. 12.1,

$$\beta_0 = \beta - f_{N(\beta)}\,; \quad -u_{N(\beta)} \leq f_{N(\beta)} \leq u_{N(\beta)}\,. \tag{12.6}$$

Clearly, whenever $N(\beta)$ is used, its true value β_0 will be effective. In linking up a standard β_1 of true value $\beta_{0,1}$ to $N(\beta)$, the physical error equation reads

$$\beta_{1,l} = \beta_0 + x_l = \beta_0 + x_0 + (x_l - \mu_x) + f_x\,; \quad l = 1, \ldots, n\,.$$

Obviously, β_0 and x_0 define the true value

$$\beta_{0,1} = \beta_0 + x_0 \tag{12.7}$$

of the standard β_1. Averaging over the n values $\beta_{1,l}$; $l = 1, \ldots, n$ leads to

$$\bar{\beta}_1 = \beta_0 + \bar{x}\,. \tag{12.8}$$

Unfortunately, the so-defined quantity is metrologically undefined. In order to arrive at a useful statement, we have to substitute $N(\beta)$ for β_0 and include the associated systematic error $f_{N(\beta)}$ into the uncertainty of the modified mean

$$\bar{\beta}_1 = N(\beta) + \bar{x} \tag{12.9}$$

so that

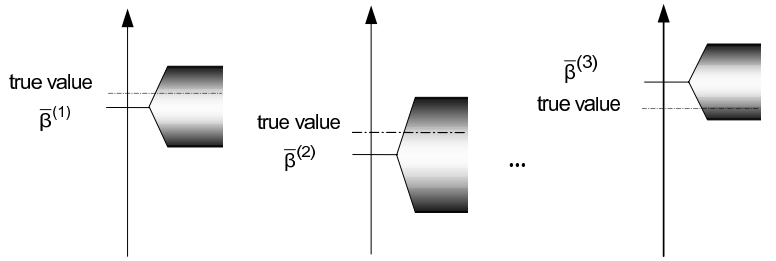


Fig. 12.2. The true values of standards of same hierarchical rank need not coincide, nor must their uncertainties overlap – the respective uncertainties should rather localize the associated true values

$$u_{\bar{\beta}_1} = u_{N(\beta)} + \frac{t_P(n-1)}{\sqrt{n}} s_{\bar{x}} + f_{s,x}\,. \tag{12.10}$$

According to

$$\bar{\beta}_1 - u_{\bar{\beta}_1} \le \beta_{0,1} \le \bar{\beta}_1 + u_{\bar{\beta}_1}\,, \tag{12.11}$$

the interval $\bar{\beta}_1 \pm u_{\bar{\beta}_1}$ localizes the true value $\beta_{0,1}$ of the lower-ranking standard $\bar{\beta}_1$. The true value $\beta_{0,1}$ of $\bar{\beta}_1$ will, of course, differ from the true value β_0 of the primary standard $N(\beta)$.

12.1.2 Key Comparison

So-called key comparisons shall ensure the national measurement institutes to rely on equivalent SI standards. Let $\bar{\beta}^{(1)}, \bar{\beta}^{(2)}, \ldots, \bar{\beta}^{(m)}$ denote a selected group of standards (of equal physical quality) with true values $\beta_0^{(i)}$; $i = 1, \ldots, m$. The superscripts distinguish individuals of the same hierarchical rank, Fig. 12.2. Again, the true values of the standards need not coincide. It is rather indispensable that the uncertainties of the standards localize the respective true values. Key comparisons are implemented through round robins in which a suitable transfer standard, which we shall call T, is passed on from one participant to the next where it is calibrated on the spot, Fig. 12.3. During the portage the physical properties of the transfer standard must not alter so that each link-up relates exactly to one and the same true value. Subsequently, the mutual consistency of the results has to be tested.

The i-th participant, $i \in 1, \ldots, m$, links the transfer standard T to his laboratory standard $\bar{\beta}^{(i)}$. We assume the uncertainties of the laboratory standards to localize the pertaining true values $\beta_0^{(i)}$ so that

$$\bar{\beta}^{(i)} - u_{\bar{\beta}^{(i)}} \le \beta_0^{(i)} \le \bar{\beta}^{(i)} + u_{\bar{\beta}^{(i)}}\,, \quad i = 1, \ldots, m\,. \tag{12.12}$$

For convenience, let us rewrite these inequalities as a set of equations

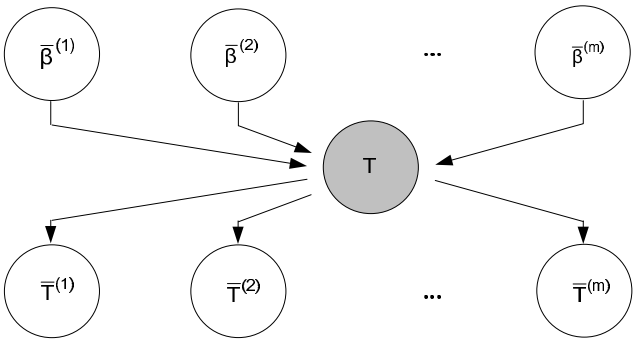


Fig. 12.3. Round robin for a group of m standards $\boldsymbol{\beta}^{(i)}$; $i = 1, \ldots, m$ realized by means of a transfer standard T. The calibrations $\bar{T}^{(i)}$ should be mutually consistent

$$\bar{\beta}^{(i)} = \beta_0^{(i)} + f_{\bar{\beta}^{(i)}}\,; \quad -u_{\bar{\beta}^{(i)}} \le f_{\bar{\beta}^{(i)}} \le u_{\bar{\beta}^{(i)}}\,; \quad i = 1, \ldots, m\,. \tag{12.13}$$

The physical error equations of the m link-ups read

$$T_l^{(i)} = \beta_0^{(i)} + x_0^{(i)} + \left(x_l^{(i)} - \mu_{x^{(i)}}\right) + f_{x^{(i)}}\,; \quad i = 1, \ldots, m\,; \quad l = 1, \ldots, n$$
$$\bar{T}^{(i)} = \beta_0^{(i)} + x_0^{(i)} + \left(\bar{x}^{(i)} - \mu_{x^{(i)}}\right) + f_{x^{(i)}}\,; \quad i = 1, \ldots, m\,.$$

The second group of equations is obviously identical to

$$\bar{T}^{(i)} = \beta_0^{(i)} + \bar{x}^{(i)}\,; \quad i = 1, \ldots, m\,.$$

For practical reasons, we have to substitute estimators $\bar{\beta}^{(i)}$ for the inaccessible true values $\beta_0^{(i)}$ and to include the imported errors in the uncertainty $u_{\bar{T}^{(i)}}$ of the relevant mean $\bar{T}^{(i)}$. We then find

$$\bar{T}^{(i)} = \bar{\beta}^{(i)} + \bar{x}^{(i)}\,, \quad u_{\bar{T}^{(i)}} = u_{\bar{\beta}^{(i)}} + u_{\bar{x}^{(i)}}\,; \quad i = 1, \ldots, m\,. \tag{12.14}$$

Let T_0 designate the true value of the transfer standard. As

$$T_0 = \beta_0^{(i)} + x_0^{(i)}\,; \quad i = 1, \ldots, m\,, \tag{12.15}$$

we have

$$\left|\bar{T}^{(i)} - T_0\right| \le u_{\bar{T}^{(i)}}\,; \quad i = 1, \ldots, m\,. \tag{12.16}$$

Figure 12.4 depicts the result of a consistent round robin.

We might wish to quantify differences of the kind $\bar{T}^{(i)} - \bar{T}^{(j)}$. Here, we should observe

$$\left|\bar{T}^{(i)} - \bar{T}^{(j)}\right| \le u_{\bar{\beta}^{(i)}} + u_{\bar{x}^{(i)}} + u_{\bar{\beta}^{(j)}} + u_{\bar{x}^{(j)}}\,; \quad i = 1, \ldots, m\,.$$

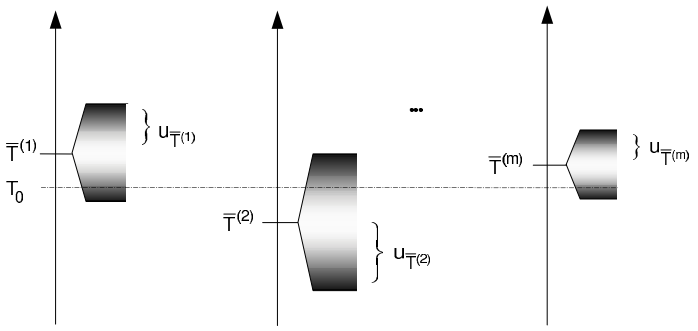


Fig. 12.4. Round robin: in case of consistency of the standards $\bar{\beta}^{(i)}$; $i = 1, \ldots, m$, a horizontal line may be drawn intersecting each of the uncertainties $u_{\bar{T}^{(i)}}$ of the calibrations $\bar{T}^{(i)}$

Finally, we refer to the m means $\bar{T}^{(i)}$ to establish a weighted grand mean[1] as defined in (9.41),

$$\bar{\beta} = \sum_{i=1}^{m} w_i \bar{T}^{(i)}\,; \quad w_i = \frac{g_i^2}{\sum\limits_{i=1}^{m} g_i^2}\,; \quad g_i = \frac{1}{u_{\bar{T}^{(i)}}}\,. \tag{12.17}$$

In this context, the mean $\bar{\beta}$ is called a key comparison reference value (KCRV). We derive the uncertainties $u_{\bar{d}_i}$ of the m differences

$$\bar{d}_i = \bar{T}^{(i)} - \bar{\beta}\,; \quad i = 1, \ldots, m\,. \tag{12.18}$$

To this end, we have to insert (12.14) into (12.18), so that

$$\bar{d}_i = \bar{\beta}^{(i)} + \bar{x}^{(i)} - \sum_{j=1}^{m} w_j \left(\bar{\beta}^{(j)} + \bar{x}^{(j)}\right)\,.$$

Combining the two errors $f_{x^{(i)}}$ and $f_{\bar{\beta}^{(i)}}$

$$f_i = f_{x^{(i)}} + f_{\bar{\beta}^{(i)}}\,, \tag{12.19}$$

the error representation of (12.18) reads

$$\begin{aligned}\bar{d}_i &= T_0 + \left(\bar{x}^{(i)} - \mu_{x^{(i)}}\right) + f_i - \sum_{j=1}^{m} w_j \left[T_0 + \left(\bar{x}^{(j)} - \mu_{x^{(j)}}\right) + f_j\right] \\ &= \left(\bar{x}^{(i)} - \mu_{x^{(i)}}\right) - \sum_{j=1}^{m} w_j \left(\bar{x}^{(j)} - \mu_{x^{(j)}}\right) + f_i - \sum_{j=1}^{m} w_j f_j\,. \end{aligned} \tag{12.20}$$

[1] As has been discussed in Sect. 9.3, a group of means with unequal true values does not define a coherent grand mean.

Reverting to individual measurements $x_l^{(i)}$ we find

$$\bar{d}_i = \frac{1}{n}\sum_{l=1}^{n}\left(x_l^{(i)} - \mu_{x^{(i)}}\right) - \sum_{j=1}^{m} w_j \left[\frac{1}{n}\sum_{l=1}^{n}\left(x_l^{(j)} - \mu_{x^{(j)}}\right)\right] + f_i - \sum_{j=1}^{m} w_j f_j$$

$$= \frac{1}{n}\sum_{l=1}^{n}\left[\left(x_l^{(i)} - \mu_{x^{(i)}}\right) - \sum_{j=1}^{m} w_j \left(x_l^{(j)} - \mu_{x^{(j)}}\right)\right] + f_i - \sum_{j=1}^{m} w_j f_j$$

so that

$$\bar{d}_{i,l} = \left(x_l^{(i)} - \mu_{x^{(i)}}\right) - \sum_{j=1}^{m} w_j \left(x_l^{(j)} - \mu_{x^{(j)}}\right) + f_i - \sum_{j=1}^{m} w_j f_j$$

$$l = 1, \ldots, n\,. \tag{12.21}$$

Hence, we are in a position to define the n differences

$$\bar{d}_{i,l} - \bar{d}_i = \left(x_l^{(i)} - \bar{x}^{(i)}\right) - \sum_{j=1}^{m} w_j \left(x_l^{(j)} - \bar{x}^{(j)}\right)\,, \quad l = 1, \ldots, n\,. \tag{12.22}$$

The empirical variances and covariances of the participants are

$$s_{\bar{x}^{(i)}\bar{x}^{(j)}} \equiv s_{ij} = \frac{1}{n-1}\sum_{l=1}^{n}\left(x_l^{(i)} - \bar{x}^{(i)}\right)\left(x_l^{(j)} - \bar{x}^{(j)}\right)\,; \quad i, j = 1, \ldots, m\,.$$

The s_{ij} define the empirical variance–covariance matrix

$$\boldsymbol{s} = \begin{pmatrix} s_{11} & s_{12} & \ldots & s_{1m} \\ s_{21} & s_{22} & \ldots & s_{2m} \\ \ldots & \ldots & \ldots & \ldots \\ s_{m1} & s_{m2} & \ldots & s_{mm} \end{pmatrix}\,; \quad s_{ii} \equiv s_i^2\,.$$

For convenience, we introduce the auxiliary vector

$$\boldsymbol{w} = (w_1\, w_2\, \ldots\, w_m)^{\mathrm{T}}$$

comprising the weights w_i. Then, from (12.22) we obtain

$$s_{\bar{d}_i}^2 = \frac{1}{n-1}\sum_{l=1}^{n}\left(\bar{d}_{i,l} - \bar{d}_i\right)^2 = s_i^2 - 2\sum_{j=1}^{m} w_j s_{ij} + \boldsymbol{w}^{\mathrm{T}}\boldsymbol{s}\boldsymbol{w}\,. \tag{12.23}$$

The worst case estimation of (12.19) yields

$$f_{s,i} = f_{s,x^{(i)}} + u_{\bar{\beta}^{(i)}}\,; \quad i = 1, \ldots, m\,.$$

Hence, the uncertainties of the differences (12.18) are given by

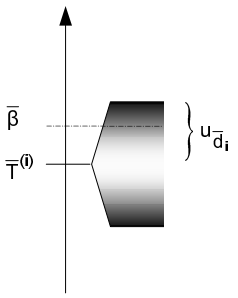


Fig. 12.5. The absolute value of the difference $\bar{d}_i = \bar{T}^{(i)} - \bar{\beta}$ should not exceed the uncertainty $u_{\bar{d}_i}$

$$u_{\bar{d}_i} = \frac{t_P(n-1)}{\sqrt{n}} \sqrt{s_i^2 - 2\sum_{j=1}^{m} w_j s_{ij} + \boldsymbol{w}^{\mathrm{T}} \boldsymbol{s} \boldsymbol{w}}$$
$$+ (1 - w_i)\, f_{s,i} + \sum_{j=1 j \neq i}^{m} w_j f_{s,j}\,, \quad i = 1, \ldots, m\,.$$

We are free to add to the second term on the right $\pm w_i f_{s,i}$,

$$(1 - w_i)\, f_{s,i} + \sum_{j=1 j \neq i}^{m} w_j f_{s,j} \pm w_i f_{s,i} = f_{s,i} - 2 w_i f_{s,i} + \sum_{j=1}^{m} w_j f_{s,j}\,,$$

so that

$$u_{\bar{d}_i} = \frac{t_P(n-1)}{\sqrt{n}} \sqrt{s_i^2 - 2\sum_{j=1}^{m} w_j s_{ij} + \boldsymbol{w}^{\mathrm{T}} \boldsymbol{s} \boldsymbol{w}}$$
$$+ f_{s,i} - 2 w_i f_{s,i} + \sum_{j=1}^{m} w_j f_{s,j}\,. \tag{12.24}$$

As illustrated in Fig. 12.5, we should observe

$$\left| \bar{T}^{(i)} - \bar{\beta} \right| \leq u_{\bar{d}_i}\,. \tag{12.25}$$

In case of equal weights, we have to set $w_i = 1/m$. Whether or not (12.25) turns out to be practically useful, appears somewhat questionable. Let us recall that the grand mean $\bar{\beta}$ as defined in (12.17) is established through the calibrations $\bar{T}^{(i)}$ themselves. Consequently, we cannot rule out that just by chance, correct calibrations might appear to be incorrect and incorrect ones to appear correct.

Rather, it appears simpler and less risky to check whether the uncertainties of the $\bar{T}^{(i)}$; $i = 1, \ldots, m$ mutually overlap. If they do, this would indicate compatibility of the $\bar{\beta}^{(1)}, \bar{\beta}^{(2)}, \ldots, \bar{\beta}^{(m)}$.

Finally, let us refer to what metrologists call "traceability". In a sense, this is the most basic definition of metrology stating the imperative: the uncertainty of every standard and every physical quantity should localize the pertaining true value. Provided the alternative error model we refer to applies, we are in a position to claim:

The alternative error model meets the requirements of traceability.

In contrast to this, the *ISO Guide* presents us with difficulties of how to explain the term and of how to realize its implications – even lengthy discussions holding up for years do not seem to have clarified the situation.

12.2 Mass Decades

Since the First General Conference of Weights and Measures in 1889, the unit of mass is realized through artefacts, namely so-called prototypes of the kilogram.[2] However, as thorough long-term investigations have revealed, mass artefacts are not really time-constant quantities. Their inconstancies might amount up to $\pm 5\,\mu g$ [15]. Another problem relates to the high density of the platinum-iridium alloy. Their density of $21\,500\,kg\,m^{-3}$ has to be confronted with the density of $8\,000\,kg\,m^{-3}$ of stainless steel weights. According to this difference, the primary link-up

$$\text{prototype} \quad \Rightarrow \quad 1\,\text{kg stainless steel weight}$$

is affected by an air buoyancy of the order of magnitude of 100 mg, the uncertainty of which should lie in an interval of $\pm 5\,\mu g$ up to $\pm 10\,\mu g$.

The scaling of the kilogram, there are submultiples and multiples as

$$\ldots, 10\,g\,,\ 20\,g\,,\ 50\,g\,,\ 100\,g\,,\ 200\,g\,,\ 500\,g\,,\ 1\,kg\,,\ 2\,kg\,,\ 5\,kg\,,\ \ldots \quad (12.26)$$

is carried out through weighing. In the following, we shall consider the ideas underlying mass link-ups. To adjust the weights to exact nominal values would be neither necessary nor, regarding the costs, desirable. Rather, differences of the kind

$$\beta_k = m_k - N(m_k)\,; \quad k = 1, 2, \ldots \quad (12.27)$$

between the physical masses m_k and their nominal values $N(m_k)$ are considered.

Weighing Schemes

For simplicity, we shall confine ourselves to "down-scaling". Consider a set of weights with nominal values

[2] The prototypes, whose nominal value is 1 kg (exact), are cylinders 39 mm in height and 39 mm in diameter and consist of an alloy of 90% platinum and 10% iridium. At present, a new definition of the SI unit kg is being investigated.

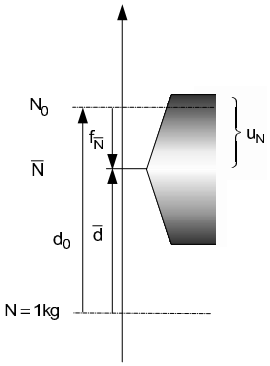


Fig. 12.6. Link-up standard with nominal value N, true value N_0 and mean value $\bar{N}$

$$N(m_1) = 500\,\mathrm{g}\,, \quad N(m_2) = 200\,\mathrm{g}\,, \quad N(m_3) = 200\,\mathrm{g}$$
$$N(m_4) = 100\,\mathrm{g}\,, \quad N(m_5) = 100\,\mathrm{g}\,. \tag{12.28}$$

In order to better control the weighing procedures, we might wish to add a so-called check-weight, for example

$$N(m_6) = 300\,\mathrm{g}\,,$$

the actual mass of which is known a priori. After the link-up, the two intervals

$$(\bar{m}_6 \pm u_{\bar{m}_6})_{\text{before calibration}} \qquad (\bar{m}_6 \pm u_{\bar{m}_6})_{\text{after calibration}}$$

should mutually overlap.

According to Fig. 12.6, we assume that a standard of nominal value $N = 1\,\mathrm{kg}$ is provided, N_0 being its physically true value, and $\bar{N}$ its known mean value with uncertainty $u_{\bar{N}}$,

$$\bar{N} - u_{\bar{N}} \le N_0 \le \bar{N} + u_{\bar{N}}\,; \quad \bar{N} = N_0 + f_{\bar{N}}\,; \quad -u_{\bar{N}} \le f_{\bar{N}} \le u_{\bar{N}}\,. \tag{12.29}$$

We shall always liken two groups of weights of equal nominal values, e.g.

$$\left.\begin{array}{lll} \{m_1 + m_2 + m_3 + m_6\} & \text{nominal value} & 1.2\,\mathrm{kg} \\ \{m_4 + m_5 + N_0\} & \text{nominal value} & 1.2\,\mathrm{kg} \end{array}\right\} \quad \text{1st comparison}\,.$$

We refer to $l = 1, \ldots, n$ repeat measurements and represent the comparison in the form of an observational equation

$$\{m_1 + m_2 + m_3 + m_6\} - \{m_4 + m_5 + N_0\} \approx \bar{x}_1\,; \quad \bar{x}_1 = \frac{1}{n}\sum_{l=1}^{n} x_{1,l}\,.$$

In physical terms, the link-up standard enters, of course, with its true value N_0. As this value is unknown, we have to substitute $\bar{N}$ for N_0 and to increase the uncertainty $u_{\bar{x}_1}$ of the right-hand side by $u_{\bar{N}}$ up to $u_{\bar{N}} + u_{\bar{x}_1}$,

$$\{m_1 + m_2 + m_3 + m_6\} - \{m_4 + m_5 + \bar{N}\} \approx \bar{x}_1$$
$$u_{\text{right-hand side}} = u_{\bar{N}} + u_{\bar{x}_1} .$$

For convenience, we now turn to deviations as defined in (12.27),

$$\beta_1 + \beta_2 + \beta_3 - \beta_4 - \beta_5 + \beta_6 \approx \bar{x}_1 + \bar{d} . \tag{12.30}$$

Here

$$\bar{d} = \bar{N} - N \tag{12.31}$$

denotes the difference between $\bar{N}$ and N, obviously,

$$d_0 = N_0 - N \tag{12.32}$$

denotes the true value of $\bar{d}$. The associated error equation is

$$\bar{d} = d_0 + f_{\bar{N}} ; \quad -u_{\bar{N}} \leq f_{\bar{N}} \leq u_{\bar{N}} . \tag{12.33}$$

As we learn from (12.30), the first row of the design matrix $\boldsymbol{A}$ are numbers $+1$ or -1, depending on whether the weight is a member of the first or of the second group. Since there are also comparisons which do not include all weights of the set considered, e.g.

$$\left.\begin{array}{lll} \{m_6\} & \text{nominal value} & 300\,\text{g} \\ \{m_3 + m_5\} & \text{nominal value} & 300\,\text{g} \end{array}\right\} \quad \text{2nd comparison} ,$$

i.e.

$$-\beta_3 - \beta_5 + \beta_6 \approx \bar{x}_2 ,$$

there will also be zeros. The first two rows of the design matrix $\boldsymbol{A}$ read

$$\begin{array}{cccccc} 1 & 1 & 1 & -1 & -1 & 1 \\ 0 & 0 & -1 & 0 & -1 & 1 \end{array} . \tag{12.34}$$

If there are r unknowns β_k; $k = 1, \ldots, r$ we need $m > r$ observational equations, allowing for $\text{rank}(\boldsymbol{A}) = r$.

The exemplary weighing scheme presented below is made up of $m = 16$ mass comparisons and $r = 6$ unknown weights. The first five comparisons include the link-up standard $\bar{N}$, which in the design matrix is indicated by a $(+)$ sign. In general, $\bar{N}$ will appear within the first p observational equations so that

$$\bar{\boldsymbol{d}} = (\underbrace{\bar{d} \ldots \bar{d}}_{p} \,|\, \underbrace{0 \ldots 0}_{m-p})^{\mathrm{T}} . \tag{12.35}$$

Furthermore, 14 comparisons include the check-weight. Setting

$$\boldsymbol{\beta} = (\beta_1\, \beta_2\, \ldots\, \beta_r)^{\mathrm{T}} , \quad \bar{\boldsymbol{x}} = (\bar{x}_1\, \bar{x}_2\, \ldots\, \bar{x}_m)^{\mathrm{T}} ,$$

$$\boldsymbol{A} = \begin{pmatrix} 1 & 1 & 1 & -1 & -1 & 1 \\ 1 & -1 & 1 & 1 & 1 & 1 \\ 1 & 1 & -1 & 1 & 1 & 1 \\ 1 & 1 & 0 & 1 & -1 & 1 \\ 1 & 0 & 1 & -1 & 1 & 1 \\ 1 & -1 & 1 & -1 & -1 & -1 \\ 1 & -1 & -1 & 1 & 1 & -1 \\ 1 & 1 & -1 & -1 & -1 & -1 \\ 1 & -1 & 0 & 1 & -1 & -1 \\ 1 & 0 & -1 & -1 & 1 & -1 \\ 0 & -1 & 0 & -1 & 0 & 1 \\ 0 & -1 & 0 & -1 & 0 & 1 \\ 0 & 0 & -1 & 0 & -1 & 1 \\ 0 & 0 & -1 & 0 & -1 & 1 \\ 0 & 0 & 0 & 1 & -1 & 0 \\ 0 & 0 & 0 & 1 & -1 & 0 \end{pmatrix} \begin{matrix} (+) \\ (+) \\ (+) \\ (+) \\ (+) \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \end{matrix}$$

the inconsistent linear system takes the form

$$\boldsymbol{A}\boldsymbol{\beta} \approx \bar{\boldsymbol{x}} + \bar{\boldsymbol{d}} . \tag{12.36}$$

The least squares solution vector is

$$\begin{aligned} \bar{\boldsymbol{\beta}} &= \left(\boldsymbol{A}^{\mathrm{T}}\boldsymbol{A}\right)^{-1} \boldsymbol{A}^{\mathrm{T}} \left(\bar{\boldsymbol{x}} + \bar{\boldsymbol{d}}\right) = \boldsymbol{B}^{\mathrm{T}} \left(\bar{\boldsymbol{x}} + \bar{\boldsymbol{d}}\right) \\ \boldsymbol{B} &= \boldsymbol{A} \left(\boldsymbol{A}^{\mathrm{T}}\boldsymbol{A}\right)^{-1} = (b_{ik}) \end{aligned} \tag{12.37}$$

or, written in components,

$$\bar{\beta}_k = \sum_{i=1}^{m} b_{ik}\bar{x}_i + \bar{d} \sum_{i=1}^{p} b_{ik} ; \quad k = 1, \ldots, r . \tag{12.38}$$

Inserting the error equations

$$\bar{x}_i = x_{0,i} + (\bar{x}_i - \mu_i) + f_i , \quad \bar{d} = d_0 + f_{\bar{N}}$$

we find

$$\bar{\beta}_k = \sum_{i=1}^{m} b_{ik} \left[x_{0,i} + (\bar{x}_i - \mu_i) + f_i\right] + (d_0 + f_{\bar{N}}) \sum_{i=1}^{p} b_{ik} ; \quad k = 1, \ldots, r .$$

Obviously,

$$\bar{\beta}_{0,k} = \sum_{i=1}^{m} b_{ik} x_{0,i} + d_0 \sum_{i=1}^{p} b_{ik} \tag{12.39}$$

are the true values of the estimators $\bar{\beta}_k$. The propagated systematic errors turn out to be

$$f_{s,\bar{\beta}_k} = \sum_{i=1}^{m} |b_{ik}|\, f_{s,i} + u_{\bar{N}} \left| \sum_{i=1}^{p} b_{ik} \right| ; \quad k = 1, \ldots, r\,. \tag{12.40}$$

Going back to individual measurements, (12.38) leads us to

$$\bar{\beta}_{kl} = \sum_{i=1}^{m} b_{ik} x_{il} + \bar{d} \sum_{i=1}^{p} b_{ik}\,; \quad k = 1, \ldots, r\,. \tag{12.41}$$

By means of the differences

$$\bar{\beta}_{kl} - \bar{\beta}_k = \sum_{i=1}^{m} b_{ik} \left(x_{il} - \bar{x}_i\right) ; \quad k = 1, \ldots, r\,; \quad l = 1, \ldots, n$$

we arrive at the empirical variances and covariances of the components of the solution vector,

$$\begin{aligned} s_{\beta_k \beta_{k'}} &= \frac{1}{n-1} \sum_{l=1}^{n} \left(\bar{\beta}_{kl} - \bar{\beta}_k\right) \left(\bar{\beta}_{k'l} - \bar{\beta}_{k'}\right) \\ &= \frac{1}{n-1} \sum_{l=1}^{n} \left[\sum_{i=1}^{m} b_{ik} \left(x_{il} - \bar{x}_i\right)\right] \left[\sum_{j=1}^{m} b_{jk'} \left(x_{j\,l} - \bar{x}_j\right)\right] \\ &= \sum_{i,j}^{m} b_{ik} b_{jk'} s_{ij}\,; \quad s_{\beta_k \beta_k} \equiv s^2_{\bar{\beta}_k}\,. \end{aligned} \tag{12.42}$$

Here, the elements

$$s_{ij} = \frac{1}{n-1} \sum_{l=1}^{n} \left(x_{il} - \bar{x}_i\right) \left(x_{j\,l} - \bar{x}_j\right) ; \quad i, j = 1, \ldots, m \tag{12.43}$$

designate the empirical variances and covariances of the input data. After all, we shall assign uncertainties

$$\begin{aligned} u_{\bar{\beta}_k} &= \frac{t_P(n-1)}{\sqrt{n}} s_{\bar{\beta}_k} + f_{s,\bar{\beta}_k}\,; \quad k = 1, \ldots, r \\ &= \frac{t_P(n-1)}{\sqrt{n}} \sqrt{\sum_{i,j}^{m} b_{ik} b_{jk} s_{ij}} + \sum_{i=1}^{m} |b_{ik}|\, f_{s,i} + f_{s,\bar{N}} \sum_{i=1}^{p} |b_{ik}| \end{aligned} \tag{12.44}$$

to the r adjusted weights $\bar{\beta}_k$; $k = 1, \ldots, r$ of the set.

12.3 Pairwise Comparisons

Occasionally, within a set of physical quantities of the same quality (lengths, voltages, etc.) only differences between two individuals are measurable. Consider, for example, four quantities β_k; $k = 1, \ldots, 4$. Then, there are either six or twelve measurable differences, depending on whether not only the differences

$$(\beta_i - \beta_j) \quad \text{but also the inversions} \quad (\beta_j - \beta_i)$$

appear to be of metrological relevance. Let us refer to the first, simpler situation,

$$\begin{aligned}
\beta_1 - \beta_2 &\approx \bar{x}_1 \\
\beta_1 - \beta_3 &\approx \bar{x}_2 \\
\beta_1 - \beta_4 &\approx \bar{x}_3 \\
\beta_2 - \beta_3 &\approx \bar{x}_4 \\
\beta_2 - \beta_4 &\approx \bar{x}_5 \\
\beta_3 - \beta_4 &\approx \bar{x}_6 \,.
\end{aligned} \tag{12.45}$$

Obviously, the first and the second relation establish the fourth one, the first and the third the fifth one and, finally, the second and the third the sixth one. Consequently, the design matrix

$$\boldsymbol{A} = \begin{pmatrix}
1 & -1 & 0 & 0 \\
1 & 0 & -1 & 0 \\
1 & 0 & 0 & -1 \\
0 & 1 & -1 & 0 \\
0 & 1 & 0 & -1 \\
0 & 0 & 1 & -1
\end{pmatrix} \tag{12.46}$$

has rank 3. As has been outlined in Sect. 7.3, a constraint is needed. Let us e.g. consider

$$h_1\beta_1 + h_2\beta_2 + h_3\beta_3 + h_4\beta_4 = y \,. \tag{12.47}$$

The uncertainties of the $\bar{\beta}_k$; $k = 1, \ldots, 4$ follow from Chap. 9. Of course, the right hand side of (12.47) may also refer to quantities of the kind $\bar{y} \pm u_{\bar{y}}$.

12.4 Fundamental Constants of Physics

Among others, the following physical constants are at present considered fundamental:

h	Planck constant	R_∞	Rydberg constant
e	elementary charge	μ_B	Bohr magneton
c	speed of light in vacuum	μ_N	nuclear magneton
μ_0	permeability of vacuum	m_e	electron mass
ε_0	permittitivity of vacuum	m_p	proton mass
α	fine-structure constant	M_p	proton molar mass
γ_p	proton gyromagnetic ratio	μ_p	proton magnetic moment
N_A	Avogadro constant	F	Faraday constant

Due to measurement errors, fundamental constants taken from measured data prove mutually inconsistent, i.e. different concatenations which we expect to produce equal results, disclose numerical discrepancies. To circumvent this mishap, a sufficiently large set of constants, say r, is subjected to a least squares adjustment calling for mutual consistency. Just as the uncertainties of the input data are expected to localize the pertaining true values, we require that the adjusted constants should meet the respective demand, i.e. each of the newly obtained intervals,

$$(\text{constant} \pm \text{uncertainty})_k\,, \quad k = 1, \ldots, r$$

should localize the pertaining true value. The latter property should apply irrespective of the weighting procedure, as has been discussed in Sects. 8.4 and 9.3.

Examples of concatenations between fundamental constants are

$$R_\infty = \frac{m_\mathrm{e}}{2hc}\alpha^2\,, \quad \alpha = \frac{\mu_0 c}{2}\frac{e^2}{h}\,, \quad \mu_\mathrm{B} = \frac{eh}{4\pi m_\mathrm{e}}\,, \quad \mu_\mathrm{N} = \frac{eh}{4\pi m_\mathrm{p}}$$

$$M_\mathrm{p} = N_\mathrm{A} m_\mathrm{p}\,, \quad \gamma_\mathrm{p} = \left(\frac{\mu_\mathrm{p}}{\mu_\mathrm{B}}\right)\left(\frac{m_\mathrm{p}}{m_\mathrm{e}}\right)\frac{1}{M_\mathrm{p}} N_\mathrm{A}\, e\,, \quad \varepsilon_0\mu_0 = \frac{1}{c^2}\,, \quad F = N_\mathrm{A} e\,.$$

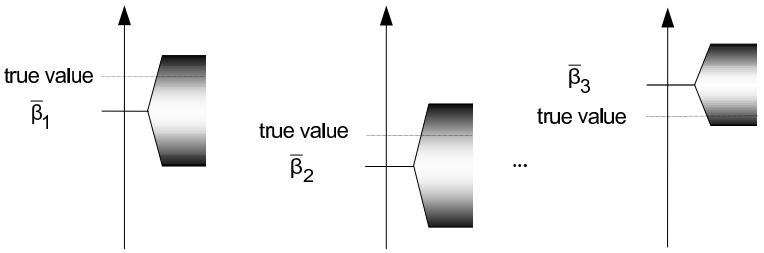
Those constants which are not members of the adjustment, will be derived from the adjusted ones so that, as the bottom line, a complete system of numerically self-consistent constants is obtained. Two remarks may be in order:

- The smaller the set of primary constants, the larger the risk of an overall maladjustment.
- The adjusted constants are not exact but rather self-consistent, i.e. they no longer give rise to numerical discrepancies.[3] We expect the uncertainties as issued by the adjustment to localize true values, Fig. 12.7

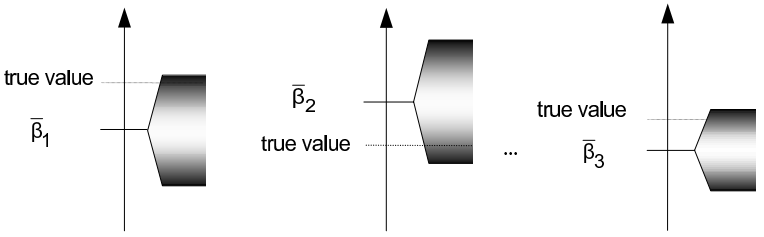
Constants may enter the adjustment either directly as measured values

$$K_i = \text{measured value} \quad (i)\,, \quad i = 1, 2, \ldots \tag{12.48}$$

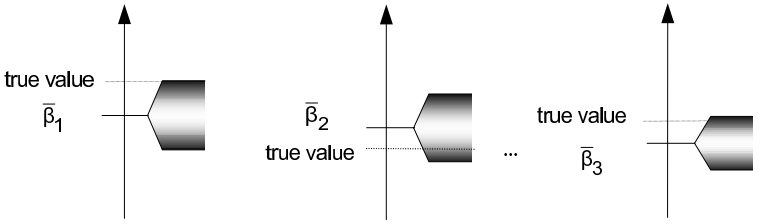
[3] I.e. the adjustment establishes consistency through redistribution of discrepancies.



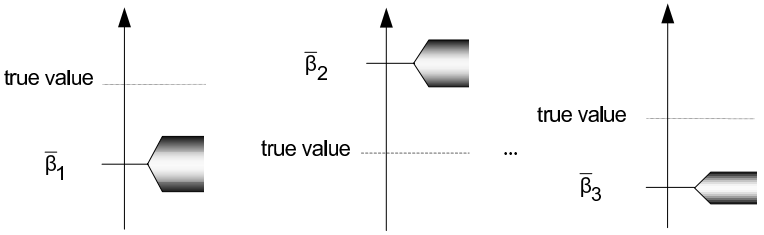
a. Even if the uncertainties of fundamental constants localize the associated true values, the constants will at least in general be numerically inconsistent.



b. Least squares shifts the values of the constants making them numerically consistent. Still, the associated uncertainties are required to localize true values.



c. Weighting the linearized system reduces the uncertainties. Given the adjustment is based on true values, the latter quantities will still be localized.



d. If, however, the adjustment is not based on true values, the result may be as illustrated here. This effect can be proved by simulation.

Fig. 12.7. Consider a set of three fundamental constants $\bar{\beta}_1$, $\bar{\beta}_2$ and $\bar{\beta}_3$ and scrutinize the interplay between weightings and the capability of the system to localize true values

or in the form of given concatenations

$$\phi_i\,(K_1, K_2, \ldots) = \text{measured value} \quad (i)\,, \quad i = 1, 2, \ldots \tag{12.49}$$

In the latter case, the functions ϕ_i, $i = 1, 2, \ldots$ have to be linearized by means of suitable starting values. The presently accepted form of adjustment is presented in [17]. Here, however, the error model recommended in [34] is used. As the latter sets aside the introduction of true values, at least in the opinion of the author, collective shifts of the numerical levels of the fundamental physical constants[4] are conceivable.

In the following, we shall outline the principles of an alternative adjustment [28].

Linearizing the System of Equations

Given m functions

$$\phi_i\,(K_1, K_2, \ldots, K_r) \approx a_i \bar{y}_i\,; \quad i = 1, \ldots, m \tag{12.50}$$

between $r < m$ constants K_k; $k = 1, \ldots, r$ to be adjusted. Not every constant will enter each functional relationship. Let the a_i be numerically known quantities the details of which will not concern us here. Furthermore, let the input data

$$\bar{y}_i = \sum_{j=1}^{m_i} w_j^{(i)} \bar{x}_j^{(i)}\,; \quad i = 1, \ldots, m \tag{12.51}$$

be weighted means, each defined through m_i means[5] $\bar{x}_j$; $j = 1, \ldots, m_i$. The quotations

$$\begin{gathered} \bar{x}_j^{(i)} \pm u_j^{(i)} \\ \bar{x}_j^{(i)} = \frac{1}{n} \sum_{l=1}^{n} x_{j\,l}^{(i)}\,, \quad u_j^{(i)} = \frac{t_P(n-1)}{\sqrt{n}} s_j^{(i)} + f_{s,j}^{(i)}\,; \quad j = 1, \ldots, m_i \end{gathered} \tag{12.52}$$

are presented by the different working groups participating in the adjustment. The pertaining error equations

$$\begin{aligned} x_{j\,l}^{(i)} &= x_0^{(i)} + \left(x_{jl}^{(i)} - \mu_j^{(i)} \right) + f_j^{(i)} \\ \bar{x}_j^{(i)} &= x_0^{(i)} + \left(\bar{x}_j^{(i)} - \mu_j^{(i)} \right) + f_j^{(i)} \\ -f_{s,j}^{(i)} &\le f_j^{(i)} \le f_{s,j}^{(i)}\,; \quad j = 1, \ldots, m_i \end{aligned} \tag{12.53}$$

[4] http://www.nist.gov

[5] See Sect. 9.3 where the precondition for the existence of metrologically reasonable mean of means has been extensively discussed.

lead us to the empirical variances and covariances of the i-th functional relationship,

$$\boldsymbol{s}^{(i)} = \left(s_{jj'}^{(i)}\right) \tag{12.54}$$
$$s_{jj'}^{(i)} = \frac{1}{n-1}\sum_{l=1}^{n}\left(x_{j\,l}^{(i)} - \bar{x}_j^{(i)}\right)\left(x_{j'l}^{(i)} - \bar{x}_{j'}^{(i)}\right); \quad s_{jj}^{(i)} \equiv {s_j^{(i)}}^2 .$$

The weights

$$w_j^{(i)} = \frac{g_j^{(i)2}}{\sum\limits_{j'=1}^{m_i} g_{j'}^{(i)2}}; \quad g_j^{(i)} = \frac{1}{u_j^{(i)}}; \quad j = 1, \ldots, m_i$$

and the uncertainties

$$u_{\bar{y}_i} = \frac{t_P(n-1)}{\sqrt{n}}\sqrt{\sum_{j,j'}^{m_i} w_j^{(i)} w_{j'}^{(i)} s_{jj'}^{(i)}} + \sum_{j}^{m_i} w_j^{(i)} f_{s,j}^{(i)} \tag{12.55}$$

have been quoted in Sect. 9.3.

Expanding the ϕ_i by means of known starting values $K_{v,k}$; $k = 1, \ldots, r$ yields

$$\phi_i\left(K_1, \ldots, K_r\right) = \phi_{i,\,v}\left(K_{v,1}, \ldots, K_{v,\,r}\right) + \frac{\partial \phi_i}{\partial K_{v,1}}\left(K_1 - K_{v,1}\right) + \cdots + \frac{\partial \phi_i}{\partial K_{v,r}}\left(K_r - K_{v,r}\right) \approx a_i \bar{y}_i .$$

Truncating non-linear terms and rearranging leads to

$$\frac{1}{\phi_{i,v}}\frac{\partial \phi_i}{\partial K_{v,1}}\left(K_1 - K_{v,1}\right) + \cdots + \frac{1}{\phi_{i,v}}\frac{\partial \phi_i}{\partial K_{v,r}}\left(K_r - K_{v,r}\right) \approx \frac{a_i \bar{y}_i - \phi_{i,v}}{\phi_{i,v}},$$

where

$$\phi_{i,v} \equiv \phi_{i,v}\left(K_{v,1}, \ldots, K_{v,r}\right) .$$

A reasonable weighting matrix is

$$\boldsymbol{G} = \operatorname{diag}\left\{g_1, g_2, \ldots, g_m\right\}; \quad g_i = \frac{1}{\left|\frac{a_i}{\phi_{i,v}}\right| \bar{u}_{y_i}}, \tag{12.56}$$

leading to

$$\frac{g_i}{\phi_{i,\,v}}\frac{\partial \phi_i}{\partial K_{v,1}}\left(K_1 - K_{v,1}\right) + \cdots + \frac{g_i}{\phi_{i,v}}\frac{\partial \phi_i}{\partial K_{v,r}}\left(K_r - K_{v,r}\right) \approx g_i \frac{a_i \bar{y}_i - \phi_{i,v}}{\phi_{i,v}}$$
$$i = 1 \ldots, m . \tag{12.57}$$

To abbreviate, we put

$$K_k - K_{v,k} = K_{v,k}\beta_k\,; \quad K_{v,k}\frac{g_i}{\phi_{i,v}}\frac{\partial\phi_i}{\partial K_{v,k}} = a_{ik}\,; \quad \bar{z}_i = g_i\frac{a_i\bar{y}_i - \phi_{i,v}}{\phi_{i,v}} \tag{12.58}$$

so that (12.57) turns into

$$a_{i1}\beta_1 + \cdots + a_{ir}\beta_r \approx \bar{z}_i\,; \quad i = 1,\ldots,m\,. \tag{12.59}$$

Finally, defining

$$\boldsymbol{A} = (a_{ik})\ , \quad \boldsymbol{\beta} = (\beta_1\,\beta_2\,\ldots\,\beta_r)^{\mathrm{T}} \quad \text{and} \quad \bar{\boldsymbol{z}} = (\bar{z}_1\,\bar{z}_2\,\ldots\,\bar{z}_m)^{\mathrm{T}}$$

we arrive at

$$\boldsymbol{A}\boldsymbol{\beta} \approx \bar{\boldsymbol{z}}\,. \tag{12.60}$$

Here, the $\approx$ sign implies both, linearization and measurement errors.

Structure of the Solution Vector

From (12.60) we obtain

$$\bar{\boldsymbol{\beta}} = \boldsymbol{B}^{\mathrm{T}}\bar{\boldsymbol{z}}\,; \quad \boldsymbol{B} = \boldsymbol{A}\left(\boldsymbol{A}^{\mathrm{T}}\boldsymbol{A}\right)^{-1}\,, \tag{12.61}$$

or, written in components,

$$\bar{\beta}_k = \sum_{i=1}^{m} b_{ik}\bar{z}_i\,; \quad k = 1,\ldots,r\,.$$

Inserting the $\bar{z}_i$ as given in (12.58) yields

$$\bar{\beta}_k = \sum_{i=1}^{m} b_{ik}\bar{z}_i = \sum_{i=1}^{m} b_{ik}g_i\frac{a_i\bar{y}_i - \phi_{i,\,v}}{\phi_{i,v}} = \sum_{i=1}^{m} b_{ik}g_i\frac{a_i\bar{y}_i}{\phi_{i,v}} - \sum_{i=1}^{m} b_{ik}g_i\,.$$

We then introduce the $\bar{y}_i$ according to (12.51),

$$\bar{\beta}_k = \sum_{i=1}^{m} b_{ik}\frac{a_i g_i}{\phi_{i,v}}\sum_{j=1}^{m_i} w_j^{(i)}\bar{x}_j^{(i)} - \sum_{i=1}^{m} b_{ik}g_i\,, \tag{12.62}$$

and, finally, the $\bar{x}_j^{(i)}$ as given in (12.53),

$$\begin{aligned}\bar{\beta}_k &= \sum_{i=1}^{m} b_{ik}\frac{a_i g_i}{\phi_{i,v}}\sum_{j=1}^{m_i} w_j^{(i)}\left[x_0^{(i)} + \left(\bar{x}_j^{(i)} - \mu_j^{(i)}\right) + f_j^{(i)}\right] - \sum_{i=1}^{m} b_{ik}g_i \\ &= \sum_{i=1}^{m} b_{ik}\frac{a_i g_i}{\phi_{i,v}}x_0^{(i)} - \sum_{i=1}^{m} b_{ik}g_i \\ &\quad + \sum_{i=1}^{m} b_{ik}\frac{a_i g_i}{\phi_{i,v}}\sum_{j=1}^{m_i} w_j^{(i)}\left[\left(\bar{x}_j^{(i)} - \mu_j^{(i)}\right) + f_j^{(i)}\right]\,.\end{aligned} \tag{12.63}$$

Obviously,

$$\beta_{0,k} = \sum_{i=1}^{m} b_{ik} \frac{a_i g_i}{\phi_{i,v}} x_0^{(i)} - \sum_{i=1}^{m} b_{ik} g_i = \sum_{i=1}^{m} b_{ik} g_i \frac{a_i x_0^{(i)} - \phi_{i,v}}{\phi_{i,v}}$$
$$k = 1\,, \ldots,\, r \tag{12.64}$$

designate the true values of the estimators $\bar{\beta}_k$ within the limits of vanishing linearization errors so that

$$\bar{\beta}_k = \beta_{0,k} + \sum_{i=1}^{m} b_{ik} \frac{a_i g_i}{\phi_{i,v}} \sum_{j=1}^{m_i} w_j^{(i)} \left[\left(\bar{x}_j^{(i)} - \mu_j^{(i)} \right) + f_j^{(i)} \right] . \tag{12.65}$$

From this we obtain the propagated systematic errors

$$f_{\bar{\beta}_k} = \sum_{i=1}^{m} b_{ik} \frac{a_i g_i}{\phi_{i,v}} \sum_{j=1}^{m_i} w_j^{(i)} f_j^{(i)}\,; \quad k = 1, \ldots, r\,. \tag{12.66}$$

To simplify the handling, we alter the nomenclature and transfer the double sum (12.62) into an ordinary sum,

$$\begin{aligned}
\bar{\beta}_k = \; & b_{1k} \tfrac{a_1 g_1}{\phi_{1,v}} \left[w_1^{(1)} \bar{x}_1^{(1)} + w_2^{(1)} \bar{x}_2^{(1)} + \ldots + w_{m_1}^{(1)} \bar{x}_{m_1}^{(1)} \right] \\
& + b_{2k} \tfrac{a_2 g_2}{\phi_{2,v}} \left[w_1^{(2)} \bar{x}_1^{(2)} + w_2^{(2)} \bar{x}_2^{(2)} + \ldots + w_{m_2}^{(2)} \bar{x}_{m_2}^{(2)} \right] \\
& \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots \\
& + b_{mk} \tfrac{a_m g_m}{\phi_{m,v}} \left[w_1^{(m)} \bar{x}_1^{(m)} + w_2^{(m)} \bar{x}_2^{m} + \ldots + w_{m_m}^{(m)} \bar{x}_{m_m}^{(m)} \right] - \sum_{i=1}^{m} b_{ik} g_i
\end{aligned}$$

so that

$$\bar{\beta}_k = \sum_{i=1}^{M} \tilde{b}_{ik} \bar{v}_i - \sum_{i=1}^{m} b_{ik} g_i \tag{12.67}$$

putting

$$M = \sum_{i=1}^{m} m_i \tag{12.68}$$

and

$$\begin{array}{lllllllllll}
i = 1: & \bar{v}_1 & = & \bar{x}_1^{(1)} & \bar{v}_2 & = & \bar{x}_2^{(1)} & \cdots & \bar{v}_{m_1} & = & \bar{x}_{m_1}^{(1)} \\
i = 2: & \bar{v}_{m_1+1} & = & \bar{x}_1^{(2)} & \bar{v}_{m_1+2} & = & \bar{x}_2^{(2)} & \cdots & \bar{v}_{m_1+m_2} & = & \bar{x}_{m_2}^{(2)} \\
\ldots & & & \ldots & & & \ldots & \ldots & & & \ldots \\
i = m: & \bar{v}_{q+1} & = & \bar{x}_1^{(m)} & \bar{v}_{q+2} & = & \bar{x}_2^{(m)} & \cdots & \bar{v}_M & = & \bar{x}_{m_m}^{(m)}
\end{array}$$

$$
\begin{aligned}
i=1: \quad \tilde{b}_{1k} &= b_{1k}\frac{a_1 g_1}{\phi_{1,v}}\, w_1^{(1)}\,,\\
\tilde{b}_{2k} &= b_{1k}\frac{a_1 g_1}{\phi_{1,v}}\, w_2^{(1)}\,,\\
&\cdots\cdots\cdots\cdots\\
\tilde{b}_{m_1,k} &= b_{1k}\frac{a_1 g_1}{\phi_{1,v}}\, w_{m_1}^{(1)}
\end{aligned}
$$

$$
\begin{aligned}
i=2: \quad \tilde{b}_{m_1+1,k} &= b_{2k}\frac{a_2 g_2}{\phi_{2,v}}\, w_1^{(2)}\,,\\
\tilde{b}_{m_1+2,k} &= b_{2k}\frac{a_2 g_2}{\phi_{2,v}}\, w_2^{(2)}\,,\\
&\cdots\cdots\cdots\cdots\\
\tilde{b}_{m_1+m_2,k} &= b_{2k}\frac{a_2 g_2}{\phi_{2,v}}\, w_{m_2}^{(2)}
\end{aligned}
$$

$$\cdots\cdots\cdots\cdots\cdots$$

$$
\begin{aligned}
i=m: \quad \tilde{b}_{q+1,k} &= b_{mk}\frac{a_m g_m}{\phi_{m,v}}\, w_1^{(m)}\,,\\
\tilde{b}_{q+2,k} &= b_{mk}\frac{a_m g_m}{\phi_{m,v}}\, w_2^{(m)}\,,\\
&\cdots\cdots\cdots\cdots\\
\tilde{b}_{M,k} &= b_{mk}\frac{a_m g_m}{\phi_{m,v}}\, w_{m_m}^{(m)}
\end{aligned}
$$

where

$$q=\sum_{j=1}^{m-1} m_j\,.$$

Inserting (12.52) into (12.62) yields

$$
\begin{aligned}
\bar{\beta}_k &= \sum_{i=1}^{m} b_{ik}\frac{a_i g_i}{\phi_{i,v}}\sum_{j=1}^{m_i} w_j^{(i)}\frac{1}{n}\sum_{l=1}^{n} x_{jl}^{(i)} - \sum_{i=1}^{m} b_{ik} g_i\\
&= \frac{1}{n}\sum_{l=1}^{n}\left[\sum_{i=1}^{m}\sum_{j=1}^{m_i} b_{ik}\frac{a_i g_i}{\phi_{i,v}} w_j^{(i)} x_{jl}^{(i)}\right] - \sum_{i=1}^{m} b_{ik} g_i
\end{aligned}
\tag{12.69}
$$

so that

$$\bar{\beta}_k = \sum_{i=1}^{m}\bar{\beta}_{kl}\,; \quad k=1,\ldots,r \tag{12.70}$$

understanding the

$$\bar{\beta}_{kl} = \sum_{i=1}^{m} \sum_{j=1}^{m_i} b_{ik} \frac{a_i g_i}{\phi_{i,v}} \, w_j^{(i)} x_{jl}^{(i)} - \sum_{i=1}^{m} b_{ik} g_i \, ;$$
$$k = 1, \ldots, r \, ; \quad l = 1, \ldots, n \tag{12.71}$$

as estimators of an adjustment based on the respective l-th repeat measurements. The n differences between (12.71) and (12.62),

$$\bar{\beta}_{kl} - \bar{\beta}_k = \sum_{i=1}^{m} \sum_{j=1}^{m_i} b_{ik} \frac{a_i g_i}{\phi_{i,v}} \, w_j^{(i)} \left(\bar{x}_{jl}^{(i)} - \bar{x}_j^{(i)} \right) \, ;$$
$$k = 1, \ldots, r \, ; \quad l = 1, \ldots, n \tag{12.72}$$

give rise to the elements of the empirical variance–covariance matrix of the solution vector. To have a concise notation, we introduce

$$\begin{array}{llllllll}
i = 1: & v_{1l} = x_{1l}^{(1)} & v_{2l} = x_{2l}^{(1)} & \cdots & v_{m_1,l} = x_{m_1,l}^{(1)} \\
i = 2: & v_{m_1+1,l} = x_{1l}^{(2)} & v_{m_1+2,l} = x_{2l}^{(2)} & \cdots & v_{m_1+m_2,l} = x_{m_2,l}^{(2)} \\
\cdots & \cdots & \cdots & \cdots & \cdots \\
i = m: & v_{q+1,l} = x_{1l}^{(m)} & v_{q+2,l} = x_{2l}^{(m)} & \cdots & v_{M,l} = x_{m_m,l}^{(m)}
\end{array}$$

so that

$$\bar{\beta}_{kl} - \bar{\beta}_k = \sum_{i=1}^{M} \tilde{b}_{ik} \left(v_{il} - \bar{v}_i \right) \, ; \quad k = 1, \ldots, r \, ; \quad l = 1, \ldots, n \, . \tag{12.73}$$

Further, we define an auxiliary matrix assembling the $\tilde{b}_{ik}$,

$$\tilde{\boldsymbol{B}} = \left(\tilde{b}_{ik} \right) \, . \tag{12.74}$$

Then, referring to the empirical variance–covariance matrix of all input data,

$$\boldsymbol{s} = (s_{ij}) \, ; \quad s_{ij} = \frac{1}{n-1} \sum_{l=1}^{n} \left(v_{il} - \bar{v}_i \right) \left(v_{jl} - \bar{v}_j \right)$$
$$i, j = 1, \ldots, M \, , \tag{12.75}$$

the empirical variance–covariance matrix of the solution vector $\bar{\boldsymbol{\beta}}$ turns out to be

$$\boldsymbol{s}_{\bar{\beta}} = \tilde{\boldsymbol{B}}^{\mathrm{T}} \boldsymbol{s} \tilde{\boldsymbol{B}} \, . \tag{12.76}$$

Its elements are

$$s_{\bar{\beta}_k \bar{\beta}'_{k}} = \frac{1}{n-1} \sum_{l=1}^{n} \left(\bar{\beta}_{kl} - \bar{\beta}_k\right) \left(\bar{\beta}_{k'l} - \bar{\beta}_{k'}\right)$$
$$s_{\bar{\beta}_k \bar{\beta}_k} \equiv s^2_{\bar{\beta}_k}\,; \quad k, k' = 1, \ldots, r\,. \tag{12.77}$$

To concisely present the systematic errors, we set

$$\begin{array}{lllllllllll}
i = 1: & f_1 & = & f_1^{(1)} & f_2 & = & f_2^{(1)} & \cdots & f_{m_1} & = & f_{m_1}^{(1)} \\
i = 2: & f_{m_1+1} & = & f_1^{(2)} & f_{m_1+2} & = & f_2^{(2)} & \cdots & f_{m_1+m_2} & = & f_{m_2}^{(2)} \\
\cdots & & \cdots & & & \cdots & & \cdots & & \cdots & \\
i = m: & f_{q+1} & = & f_1^{(m)} & f_{q+2} & = & f_2^{(m)} & \cdots & f_M & = & f_{m_m}^{(m)}
\end{array}$$

so that (12.66) becomes

$$f_{\bar{\beta}_k} = \sum_{i=1}^{M} \tilde{b}_{ik} f_i\,; \quad k = 1, \ldots, r\,. \tag{12.78}$$

Finally, the result of the adjustments is

$$\bar{\beta}_k \pm u_{\bar{\beta}_k}$$
$$u_{\bar{\beta}_k} = \frac{t_P(n-1)}{\sqrt{n}} s_{\bar{\beta}_k} + \sum_{i=1}^{M} \left|\tilde{b}_{ik}\right| f_{s,i}\,; \quad k = 1, \ldots, r\,. \tag{12.79}$$

Uncertainties of the Constants

According to (12.58), the constants and their uncertainties turn out to be

$$\bar{K}_k = K_{k,v}\left(\bar{\beta}_k + 1\right)\,, \quad u_{\bar{K}_k} = K_{k,v} u_{\bar{\beta}_k}\,; \quad k = 1, \ldots, r\,. \tag{12.80}$$

Cyclically repeating the adjustment with improved starting values should reduce the linearization errors. However, on account of the errors of the input data, the estimators $\bar{\beta}_k$; $k = 1, \ldots, r$ tend to oscillate after a certain number of cycles, telling us to end the iteration.

12.5 Trigonometric Polynomials

Let us look for a smoothing trigonometric polynomial to be fitted to a given empirical relationship between any two measured quantities. At first, we shall assume the model function to be unknown. After this, we shall consider the model function to be known – yet to simplify, we wish to substitute a trigonometric polynomial presuming the difference between the two functions to be negligible as compared with the error bounds of the empirical data.

For simplicity we confine ourselves to the case of error-free abscissas and erroneous ordinates,

$$(x_{0,1}, \bar{y}_1)\ , \quad (x_{0,2}, \bar{y}_2)\ , \quad \ldots \quad (x_{0,m}, \bar{y}_m)\ , \tag{12.81}$$

where we assume

$$\bar{y}_i \pm u_{\bar{y}_i}\,; \quad i = 1, \ldots, m \tag{12.82}$$

$$\bar{y}_i = \frac{1}{n}\sum_{l=1}^{n} y_{il} = y_{0,i} + (\bar{y}_i - \mu_i) + f_{y_i}\,, \quad u_{\bar{y}_i} = \frac{t_P(n-1)}{\sqrt{n}} s_{y_i} + f_{s,y_i}\,.$$

12.5.1 Unknown Model Function

We require the fitted function to intersect each of the error bars of the given pairs of data. To implement this demand, we are watching out for a well-behaving, bendable trigonometric polynomial. Let us keep in mind that if the polynomial's degree is too low, it will not be in a position to adapt itself to the details suggested by the sequence of data. If it is too high, the polynomial might follow too closely the data's pseudo-structures. Fortunately, the number of terms of a trigonometric polynomial is not overly critical. Hence, we may fix its degree by trial and error so that the fitted polynomial passes through each of the error bars and, at the same time, appropriately smoothes the empirical structure of the given data sequence.

We suppose the number of data pairs to be sufficiently large and closely spaced so that the adjustment of an empirical function appears to be physically reasonable. We are then asking for a smoothing, trigonometric polynomial

$$y(x) = \beta_1 + \sum_{k=2}^{r} \beta_k t_k(x)\,; \quad r = 3, 5, 7, \ldots < m$$

$$t_k(x) = \begin{cases} \cos\left(\dfrac{k}{2}\omega_0 x\right)\,; & k \quad \text{even} \\ \sin\left(\dfrac{k-1}{2}\omega_0 x\right)\,; & k \quad \text{odd} \end{cases} \qquad k \geq 2$$

which we intend to adjust according to least squares. To find the coefficients β_k; $k = 1, \ldots, r$ over the interval

$$\Delta X = x_{0,m} - x_{0,1}\,, \tag{12.83}$$

we define

$$t_{ik} = \begin{cases} \cos\left(\dfrac{k}{2}\omega_0 x_{0,i}\right)\,; & k \quad \text{even} \\ \sin\left(\dfrac{k-1}{2}\omega_0 x_{0,i}\right)\,; & k \quad \text{odd} \end{cases} \qquad k \geq 2\,, \quad i = 1 \ldots, m\,. \tag{12.84}$$

As is well known, trigonometric polynomials (and Fourier series) are based on auxiliary frequencies which are multiples of a basic frequency

$$\omega_0 = \frac{2\pi}{\Delta X}$$

their purpose being to keep the least squares adjustment linear.[6] After all, the inconsistent system is given by

$$\beta_1 + \beta_2 t_{i2} + \cdots + \beta_r t_{ir} \approx \bar{y}_i\,; \quad i = 1, \ldots, m \qquad r = 3, 5, 7, \ldots < m\,. \tag{12.85}$$

The design matrix

$$\boldsymbol{A} = \begin{pmatrix} 1 & t_{12} & t_{13} & \cdots & t_{1r} \\ 1 & t_{22} & t_{23} & \cdots & t_{2r} \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ 1 & t_{m2} & t_{m3} & \cdots & t_{mr} \end{pmatrix}$$

and the column vectors

$$\bar{\boldsymbol{y}} = (\bar{y}_1\, \bar{y}_2\, \cdots\, \bar{y}_m)^{\mathrm{T}}\,, \quad \boldsymbol{\beta} = (\beta_1\, \beta_2\, \cdots\, \beta_r)^{\mathrm{T}}$$

transfer (12.85) into

$$\boldsymbol{A}\boldsymbol{\beta} \approx \bar{\boldsymbol{y}}\,. \tag{12.86}$$

Assuming rank $(\boldsymbol{A}) = r$ we have

$$\bar{\boldsymbol{\beta}} = \boldsymbol{B}^{\mathrm{T}}\bar{\boldsymbol{y}}\,; \quad \boldsymbol{B} = \boldsymbol{A}\left(\boldsymbol{A}^{\mathrm{T}}\boldsymbol{A}\right)^{-1} = (b_{ik})\,. \tag{12.87}$$

The components

$$\bar{\beta}_k = \sum_{i=1}^{m} b_{ik}\bar{y}_i\,; \quad k = 1, \ldots, r \tag{12.88}$$

of the solution vector $\bar{\boldsymbol{\beta}}$ establish the adjusted polynomial

$$\bar{y}(x) = \bar{\beta}_1 + \sum_{k=2}^{r} \bar{\beta}_k t_k(x)\,; \quad r = 3, 5, 7, \ldots < m\,. \tag{12.89}$$

Since the model function is unknown, all we can do is to argue as follows: The error bars $\bar{y}_i \pm u_{\bar{y}_i}$; $i = 1, \ldots, m$ localize the true values $y_{0,i}$ of the means $\bar{y}_i$. And, as the trigonometric polynomial shall pass through each of the error bars, we have

$$|\bar{y}(x_{0,i}) - y_{0,i}| \le 2u_{\bar{y}_i}\,; \quad i = 1, \ldots, m\,. \tag{12.90}$$

[6] This suggests we also adjust the frequencies, but we would then be faced with a highly non-linear problem to which, in general, there is no solution. Remarkably enough, G. Prony, a contemporary of J. Fourier, developed a true harmonic analysis.

12.5.2 Known Model Function

Provided the difference between the known model function and the approximating trigonometric polynomial is insignificant, we may formally define a true polynomial over the interval (12.83) via the true values $(x_{0,i}, y_{0,i})$; $i = 1, \ldots, m$ of the data pairs (12.81),

$$y_0(x) = \beta_{0,1} + \sum_{k=2}^{r} \beta_{0,k} t_k(x)\,; \quad r = 3, 5, 7, \ldots < m\,. \tag{12.91}$$

Obviously, (12.91) expresses equality in a formal sense. Out of necessity, we have to keep the adjusted polynomial (12.89). Assigning the $\bar{y}_i$; $i = 1, \ldots, m$ given in (12.82) to a vector

$$\bar{\boldsymbol{y}} = \boldsymbol{y}_0 + (\bar{\boldsymbol{y}} - \boldsymbol{\mu}_y) + \boldsymbol{f}_y\,,$$

(12.87) yields

$$\bar{\boldsymbol{\beta}} = \boldsymbol{B}^{\mathrm{T}} [\boldsymbol{y}_0 + (\bar{\boldsymbol{y}} - \boldsymbol{\mu}_y) + \boldsymbol{f}_y] = \bar{\boldsymbol{\beta}}_0 + \boldsymbol{B}^{\mathrm{T}} (\bar{\boldsymbol{y}} - \boldsymbol{\mu}_y) + \boldsymbol{B}^{\mathrm{T}} \boldsymbol{f}_y\,. \tag{12.92}$$

Here, the "true solution vector"

$$\boldsymbol{\beta}_0 = (\beta_{0,1}\, \beta_{0,2}\, \cdots\, \beta_{0,r})^{\mathrm{T}}$$

provides a suitable reference to assess the fluctuations of (12.89). The vector

$$\boldsymbol{f}_{\bar{\beta}} = \boldsymbol{B}^{\mathrm{T}} \boldsymbol{f}_y\,; \quad f_{\bar{\beta}_k} = \sum_{i=1}^{m} b_{ik} f_{y_i}\,; \quad k = 1, \ldots, r \tag{12.93}$$

bears the influence of the systematic errors with respect to $\boldsymbol{\beta}_0$. Let us assume that on each of the ordinates, one and the same systematic error is superimposed

$$f_{y_i} = f_y\,, \quad -f_{s,y} \le f_{y_i} \le f_{s,y}\,; \quad i = 1, \ldots, m\,.$$

Then, the $f_{\bar{\beta}_k}$; $k = 1, \ldots, r$ have to satisfy

$$f_{\bar{\beta}_k} = \sum_{i=1}^{m} b_{ik} f_{y_i} = f_y \sum_{i=1}^{m} b_{ik}\,,$$

i.e.

$$f_{\bar{\beta}_1} = f_y \quad \text{and} \quad f_{\bar{\beta}_2} = \ldots = f_{\bar{\beta}_r} = 0 \tag{12.94}$$

as

$$\sum_{i=1}^{m} b_{i1} = 1 \quad \text{and} \quad \sum_{i=1}^{m} b_{ik} = 0\,; \quad k = 2, \ldots, r\,.$$

The polynomial coefficients $\bar{\beta}_{kl}$ of the l-th set of repeat measurements

$$y_{1l},\, y_{2l},\, \cdots,\, y_{ml}\,; \quad l = 1, \ldots, n$$

may be taken from

$$\begin{aligned}\bar{\beta}_k &= \sum_{i=1}^{m} b_{ik} \left[\frac{1}{n}\sum_{l=1}^{n} y_{il}\right] = \frac{1}{n}\sum_{l=1}^{n}\sum_{i=1}^{m} b_{ik} y_{il} \\ &= \frac{1}{n}\sum_{l=1}^{n} \bar{\beta}_{kl}\,; \quad k = 1, \ldots, r\,, \end{aligned} \tag{12.95}$$

i.e.

$$\bar{\beta}_{kl} = \sum_{i=1}^{m} b_{ik} y_{il}\,; \quad k = 1, \ldots, r\,; \quad l = 1, \ldots, n\,. \tag{12.96}$$

The differences

$$\bar{\beta}_{kl} - \bar{\beta}_k = \sum_{i=1}^{m} b_{ik}\,(y_{il} - \bar{y}_i)\;; \quad k = 1, \ldots, r\,; \quad l = 1, \ldots, n \tag{12.97}$$

give rise to the elements $s_{\bar{\beta}_k \bar{\beta}_{k'}}$; $k, k' = 1, \ldots, r$ of the empirical variance–covariance matrix $\boldsymbol{s}_{\bar{\boldsymbol{\beta}}}$ of the solution vector $\bar{\boldsymbol{\beta}}$,

$$\begin{aligned} s_{\bar{\beta}_k \bar{\beta}_{k'}} &= \frac{1}{n-1}\sum_{l=1}^{n} \left(\bar{\beta}_{kl} - \bar{\beta}_k\right)\left(\bar{\beta}_{k'l} - \bar{\beta}_{k'}\right) \\ &= \frac{1}{n-1}\sum_{l=1}^{n} \left[\sum_{i=1}^{m} b_{ik}\,(y_{il} - \bar{y}_i)\right]\left[\sum_{j=1}^{m} b_{jk'}\,(y_{jl} - \bar{y}_j)\right] \\ &= \sum_{i,j=1}^{m} b_{ik} b_{jk'} s_{ij}\,; \quad s_{\bar{\beta}_k \bar{\beta}_k} \equiv s^2_{\bar{\beta}_k}\,. \end{aligned} \tag{12.98}$$

Here, the

$$s_{ij} = \frac{1}{n-1}\sum_{l=1}^{n} (y_{il} - \bar{y}_i)\,(y_{jl} - \bar{y}_j)$$

are the empirical variances and covariances of the input data. Letting $\boldsymbol{s} = (s_{ij})$ designate the associated empirical variance–covariance matrix, (12.98) changes into

$$\boldsymbol{s}_{\bar{\boldsymbol{\beta}}} = \left(s_{\bar{\beta}_k \bar{\beta}_{k'}}\right) = \boldsymbol{B}^{\mathrm{T}} \boldsymbol{s} \boldsymbol{B}\,. \tag{12.99}$$

Finally, we find

$$\bar{\beta}_k \pm u_{\bar{\beta}_k}\,; \quad k = 1, \ldots, r \tag{12.100}$$

$$u_{\bar{\beta}_1} = \frac{t_P(n-1)}{\sqrt{n}} s_{\bar{\beta}_1} + f_{s,y}\,; \quad u_{\bar{\beta}_k} = \frac{t_P(n-1)}{\sqrt{n}} s_{\bar{\beta}_k}\,; \quad k = 2, \ldots, r\,.$$

The intervals $\bar{\beta}_k \pm u_{\bar{\beta}_k}$; $k = 1, \ldots, r$ localize the auxiliary quantities $\beta_{0,k}$.

Uncertainty Band

The l-th set of input data produces the least squares polynomial

$$\bar{y}_l(x) = \bar{\beta}_{1l} + \bar{\beta}_{2l} t_2(x) + \cdots + \bar{\beta}_{rl} t_r(x)\,; \quad l = 1, \ldots, n\,. \tag{12.101}$$

According to (12.89), we have

$$\bar{y}(x) = \frac{1}{n} \sum_{l=1}^{n} y_l(x)\,. \tag{12.102}$$

The empirical variance at the point x is given by

$$s^2_{\bar{y}(x)} = \frac{1}{n-1} \sum_{l=1}^{n} \left(y_l(x) - \bar{y}(x)\right)^2\,. \tag{12.103}$$

Within the differences

$$\begin{aligned} \bar{y}_l(x) - \bar{y}(x) &= \left(\bar{\beta}_{1l} - \bar{\beta}_1\right) + \left(\bar{\beta}_{2l} - \bar{\beta}_2\right) t_2(x) + \cdots + \left(\bar{\beta}_{rl} - \bar{\beta}_r\right) t_r(x) \\ &= \sum_{i=1}^{m} \left[b_{i1} + b_{i2} t_2(x) + \cdots + b_{ir} t_r(x)\right] \left(y_{il} - \bar{y}_i\right)\,; \quad l = 1, \ldots, n \end{aligned}$$

we assign auxiliary constants

$$c_i(x) = b_{i1} + b_{i2} t_2(x) + \cdots b_{ir} t_r(x)\,; \quad i = 1, \ldots, m \tag{12.104}$$

to the square brackets. Defining the auxiliary vector $\boldsymbol{c} = (c_1\ c_2\ \cdots\ c_m)^{\mathrm{T}}$ the empirical variance $s^2_{\bar{y}(x)}$ turns into

$$s^2_{\bar{y}(x)} = \boldsymbol{c}^{\mathrm{T}} \boldsymbol{s} \boldsymbol{c}\,. \tag{12.105}$$

Finally, the uncertainty band which is a measure of the fluctuations of the least squares polynomial with respect to the formally introduced true polynomial (12.91) is given by

$$\bar{y}(x) \pm u_{\bar{y}(x)}\,; \quad u_{\bar{y}(x)} \frac{t_P(n-1)}{\sqrt{n}} s_{\bar{y}(x)} + f_{s,y}\,. \tag{12.106}$$

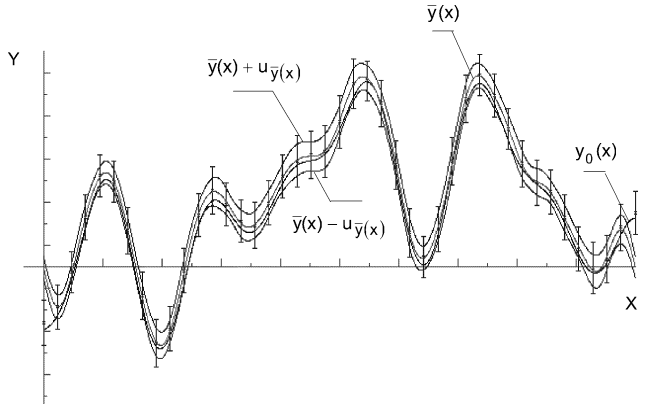


Fig. 12.8. Approximation of a given inharmonic polynomial based on five frequencies through a harmonic trigonometric least squares polynomial requiring about 16 frequencies. Data: correct abscissas, erroneous ordinates given in the form of arithmetic means

Example

Adjustment of a harmonic trigonometric polynomial.

We simplify our preconditions and assume the existence of a true known inharmonic trigonometric polynomial of the form

$$y_0(x) = a_0 + \sum_{k=1}^{N} a_k \cos \omega_k t + b_k \sin \omega_k t$$

based on $N = 5$ frequencies. We superimpose normally distributed random errors and a fixed systematic error, satisfying $f_{y_i} = f_y$; $-f_{s,y} \leq f_{y_i} \leq f_{s,y}$; $i = 1, \ldots, m$ on the ordinates of the given polynomial.

Figure 12.8 depicts the fitted harmonic trigonometric least squares polynomial and its uncertainty band.

While the given inharmonic polynomial $y_0(x)$ gets along with just $N = 5$ frequencies $\omega_1, \ldots, \omega_5$, the harmonic trigonometric least squares polynomial calls for an r of the order of magnitude 33, i.e. about 16 harmonic frequencies.

Part IV

Appendices

A On the Rank of Some Matrices

A matrix $\boldsymbol{A}$ is said to have rank r if there is at least one non-zero sub-determinant of order $(r \times r)$ while all sub-determinants of higher order are zero. The notation is rank $(\boldsymbol{A}) = r$.

The so-called design matrix $\boldsymbol{A}$, referred to in the method of least squares, Sect. 7.2, has m rows and r columns, $m > r$. Given $\boldsymbol{A}$ has rank r, its r columns are linearly independent.

It appears advantageous to regard the columns of a given matrix as vectors. Obviously, $\boldsymbol{A}$ has r m-dimensional column vectors. We denote the latter by $\boldsymbol{a}_k$; $k = 1, \ldots, r$. If the $\boldsymbol{a}_k$ are independent, they span an r-dimensional subspace $R(\boldsymbol{A}) = V_m^r(\Re)$ of the underlying m-dimensional space $V_m(\Re)$; $\Re$ denotes the set of real numbers.

1. $\boldsymbol{A}^{\mathrm{T}}\boldsymbol{A}$*, Sect. 7.2*

Let rank $(\boldsymbol{A}) = r$ and let the $\boldsymbol{a}_k$; $k = 1, \ldots, r$ be a basis of an r-dimensional subspace $R(\boldsymbol{A}) = V_m^r(\Re)$ of the m-dimensional space $V_m(\Re)$ considered. As the $\boldsymbol{a}_k$ are independent, it is not possible to find a vector

$$\boldsymbol{\beta} = (\beta_1\, \beta_2\, \cdots\, \beta_r)^{\mathrm{T}} \neq \boldsymbol{0}\,,$$

so that

$$\boldsymbol{A}\boldsymbol{\beta} = \beta_1\boldsymbol{a}_1 + \beta_2\boldsymbol{a}_2 + \cdots + \beta_r\boldsymbol{a}_r = \boldsymbol{0}\,.$$

The vector

$$\boldsymbol{c} = \beta_1\boldsymbol{a}_1 + \beta_2\boldsymbol{a}_2 + \cdots + \beta_r\boldsymbol{a}_r$$

lies in the column space of the matrix $\boldsymbol{A}$. Consequently, the vector $\boldsymbol{A}^{\mathrm{T}}\boldsymbol{c}$ must be different from the zero vector, as $\boldsymbol{c}$ cannot be orthogonal to all vectors $\boldsymbol{a}_k$; $k = 1, \ldots, r$. But, if for any vector $\boldsymbol{\beta} \neq \boldsymbol{0}$

$$\boldsymbol{A}^{\mathrm{T}}\boldsymbol{A}\boldsymbol{\beta} \neq 0\,,$$

the columns of $\boldsymbol{A}^{\mathrm{T}}\boldsymbol{A}$ are independent, i.e. rank $(\boldsymbol{A}) = r$. Moreover, as $(\boldsymbol{A}\boldsymbol{\beta})^{\mathrm{T}}\boldsymbol{A}\boldsymbol{\beta}$ equals the squared length of the vector $\boldsymbol{A}\boldsymbol{\beta}$, which is nonzero if $\boldsymbol{\beta}$ is nonzero, we have

$$\boldsymbol{\beta}^{\mathrm{T}}(\boldsymbol{A}^{\mathrm{T}}\boldsymbol{A})\boldsymbol{\beta} > 0$$

so that the symmetric matrix $\boldsymbol{A}^{\mathrm{T}}\boldsymbol{A}$ is also positive definite.

2. $\boldsymbol{B} = \boldsymbol{A}(\boldsymbol{A}^{\mathrm{T}}\boldsymbol{A})^{-1}$*, Sect. 7.2*

As $(\boldsymbol{A}^{\mathrm{T}}\boldsymbol{A})^{-1}$ is non-singular, the rank of $\boldsymbol{B}$ is that of $\boldsymbol{A}$.

3. $\boldsymbol{P} = \boldsymbol{A}(\boldsymbol{A}^{\mathrm{T}}\boldsymbol{A})^{-1}\boldsymbol{A}^{\mathrm{T}}$*, Sect. 7.2*

The rank of an idempotent matrix ($\boldsymbol{P}^2 = \boldsymbol{P}$) is equal to its trace [53]. Given that the product of two matrices, say $\boldsymbol{R}$ and $\boldsymbol{S}$, is defined in either way, $\boldsymbol{RS}$ and $\boldsymbol{SR}$, we have trace $(\boldsymbol{RS}) = \mathrm{trace}(\boldsymbol{SR})$, i.e.

$$\begin{aligned}\mathrm{rank}(\boldsymbol{P}) &= \mathrm{trace}(\boldsymbol{P}) \\ &= \mathrm{trace}\left[\boldsymbol{A}\left(\boldsymbol{A}^{\mathrm{T}}\boldsymbol{A}\right)^{-1}\boldsymbol{A}^{\mathrm{T}}\right] = \mathrm{trace}\left[\boldsymbol{A}^{\mathrm{T}}\boldsymbol{A}\left(\boldsymbol{A}^{\mathrm{T}}\boldsymbol{A}\right)^{-1}\right] = r\,.\end{aligned}$$

4. $\boldsymbol{C} = \boldsymbol{A}(\boldsymbol{A}^{\mathrm{T}}\boldsymbol{A})^{-1}\boldsymbol{H}^{\mathrm{T}}$*, Sect. 7.3*

Each of the columns of $\boldsymbol{C}$ is a linear combination of the columns of $\boldsymbol{B} = \boldsymbol{A}(\boldsymbol{A}^{\mathrm{T}}\boldsymbol{A})^{-1}$. As rank $(\boldsymbol{H}) = q$, the q columns of $\boldsymbol{C}$ are independent.

5. $\boldsymbol{B}^{\mathrm{T}}\boldsymbol{s}\boldsymbol{B}$*, Sect. 9.5*

Since we consider positive definite (non-singular) empirical variance–covariance matrices $\boldsymbol{s}$ only, we are allowed to resort to the decomposition $\boldsymbol{s} = \boldsymbol{c}^{\mathrm{T}}\boldsymbol{c}$; $\boldsymbol{c}$ denoting a non-singular $(m \times m)$ matrix [52]. As $\boldsymbol{B}^{\mathrm{T}}\boldsymbol{s}\boldsymbol{B} = (\boldsymbol{c}\,\boldsymbol{B})^{\mathrm{T}}(\boldsymbol{c}\,\boldsymbol{B})$, where rank $(\boldsymbol{c}\,\boldsymbol{B}) = r$, we have rank $(\boldsymbol{B}^{\mathrm{T}}\boldsymbol{s}\,\boldsymbol{B}) = r$. Moreover, the symmetric matrix $\boldsymbol{B}^{\mathrm{T}}\boldsymbol{s}\,\boldsymbol{B}$ is positive definite.

B Variance–Covariance Matrices

We consider m random variables X_i, $\mu_i = E\{X_i\}$; $i = 1, \ldots, m$ and m real numbers ξ_i; $i = 1, \ldots, m$. The expectation

$$E\left\{\left[\sum_{i=1}^{m} \xi_i \left(X_i - \mu_i\right)\right]^2\right\} \geq 0 \tag{B.1}$$

yields the quadratic form

$$\boldsymbol{\xi}^{\mathrm{T}} \boldsymbol{\sigma}\, \boldsymbol{\xi} \geq 0\,, \tag{B.2}$$

where

$$\boldsymbol{\xi} = \left(\xi_1\, \xi_2\, \ldots\, \xi_m\right)^{\mathrm{T}} \tag{B.3}$$

and

$$\boldsymbol{\sigma} = \begin{pmatrix} \sigma_{11} & \sigma_{12} & \ldots & \sigma_{1m} \\ \sigma_{21} & \sigma_{22} & \ldots & \sigma_{2m} \\ \ldots & \ldots & \ldots & \ldots \\ \sigma_{m1} & \sigma_{m2} & \ldots & \sigma_{mm} \end{pmatrix}$$

$$\sigma_{ij} = E\left\{\left(X_i - \mu_i\right)\left(X_j - \mu_j\right)\right\}\,; \quad i, j = 1, \ldots, m\,. \tag{B.4}$$

From (B.2) we seize: Variance–covariance matrices are at least positive semi-definite.

As the variance–covariance matrix is real and symmetric there is an orthogonal transformation for diagonalization. This in turns allows for

$$|\boldsymbol{\sigma}| = \lambda_1 \cdot \lambda_2 \cdot \ldots \cdot \lambda_m\,, \tag{B.5}$$

the λ_i; $i = 1, \ldots, m$ denoting the eigenvalues of $\boldsymbol{\sigma}$. If rank $(\boldsymbol{\sigma}) = m$, necessarily all the eigenvalues λ_i; $i = 1, \ldots, m$ are different from zero. On the other hand, given $\boldsymbol{\sigma}$ is positive definite

$$\boldsymbol{\xi}^{\mathrm{T}} \boldsymbol{\sigma}\, \boldsymbol{\xi} > 0\,, \tag{B.6}$$

the theory of quadratic forms tells us

$$\lambda_i > 0\,; \quad i = 1, \ldots, m \tag{B.7}$$

so that

$$|\boldsymbol{\sigma}| > 0\,. \tag{B.8}$$

This in the end implies: Given the the variance–covariance matrix has full rank, it is positive definite.

If (B.6) does not apply, the variance–covariance matrix $\boldsymbol{\sigma}$ is positive semi-definite, rank $(\boldsymbol{\sigma}) < m$ and some of the eigenvalues are zero, those being different from zero are still positive. We then have

$$|\boldsymbol{\sigma}| = 0\,. \tag{B.9}$$

Let us consider $m = 2$ and substitute σ_{xy} for σ_{12}; furthermore $\sigma_{xx} \equiv \sigma_x^2$ and $\sigma_{yy} \equiv \sigma_y^2$ for σ_{11} and σ_{22} respectively. Then, from

$$\boldsymbol{\sigma} = \begin{pmatrix} \sigma_{xx} & \sigma_{xy} \\ \sigma_{yx} & \sigma_{yy} \end{pmatrix}\,, \quad \text{given} \quad |\boldsymbol{\sigma}| > 0$$

we deduce

$$-\sigma_x \sigma_y < \sigma_{xy} < \sigma_x \sigma_y\,.$$

Let us now switch from expectations and theoretical variance–covariance matrices to sums and empirical variance–covariance matrices. To this end, we consider m arithmetic means

$$\bar{x}_i = \frac{1}{n} \sum_{l=1}^{n} x_{il}\,; \quad i = 1, \ldots, m\,, \tag{B.10}$$

each covering n repeat measurements x_{il}; $i = 1, \ldots, m$; $l = 1, \ldots, n$. The non-negative sum

$$\frac{1}{n-1} \sum_{l=1}^{n} \left[\sum_{i=1}^{m} \xi_i \left(x_{il} - \bar{x}_i \right) \right]^2 \geq 0 \tag{B.11}$$

yields

$$\boldsymbol{\xi}^{\mathrm{T}} \boldsymbol{s} \boldsymbol{\xi} \geq 0\,, \tag{B.12}$$

where

$$\boldsymbol{s} = \begin{pmatrix} s_{11} & s_{12} & \ldots & s_{1m} \\ s_{21} & s_{22} & \ldots & s_{2m} \\ \ldots & \ldots & \ldots & \ldots \\ s_{m1} & s_{m2} & \ldots & s_{mm} \end{pmatrix}$$

$$s_{ij} = \frac{1}{n-1} \sum_{l=1}^{n} \left(x_{il} - \bar{x}_i \right) \left(x_{j\,l} - \bar{x}_j \right)\,; \quad i, j = 1, \ldots, m \tag{B.13}$$

denotes the empirical variance–covariance matrix of the m data sets x_{il}; $i = 1, \ldots, m$; $l = 1, \ldots, n$.

Given rank $(\boldsymbol{s}) = m$, the matrix $\boldsymbol{s}$ is positive definite,

$$\boldsymbol{\xi}^{\mathrm{T}} \boldsymbol{s} \boldsymbol{\xi} > 0\,, \quad |\boldsymbol{s}| > 0\,, \tag{B.14}$$

but for rank $(\boldsymbol{s}) < m$, the matrix $\boldsymbol{s}$ is positive semi-definite,

$$\boldsymbol{\xi}^{\mathrm{T}} \boldsymbol{s} \boldsymbol{\xi} \geq 0\,, \quad |\boldsymbol{s}| = 0\,. \tag{B.15}$$

Again, we set $m = 2$ and substitute s_{xy} for s_{12}, $s_{xx} = s_x^2$ and $s_{yy} = s_y^2$ for s_{11} and s_{22} respectively. Then, from

$$\boldsymbol{s} = \begin{pmatrix} s_{xx} & s_{xy} \\ s_{yx} & s_{yy} \end{pmatrix}\,, \quad \text{provided} \quad |\boldsymbol{s}| > 0\,,$$

we obtain

$$-s_x s_y < s_{xy} < s_x s_y\,. \tag{B.16}$$

C Linear Functions of Normal Variables

We confine ourselves to sums of two (possibly dependent) normally distributed random variables, X and Y, and refer to the nomenclature introduced in Sect. 3.2, i.e. we consider

$$Z = b_x X + b_y Y \tag{C.1}$$

and denote by $\mu_x = E\{X\}$, $\mu_y = E\{Y\}$ the expectations and by $\sigma_{xx} = E\{(X-\mu_x)^2\}$, $\sigma_{yy} = E\{(Y-\mu_y)^2\}$, $\sigma_{xy} = E\{(X-\mu_x)(Y-\mu_y)\}$ the theoretical moments of second order. As usual, we associate the variables X and Y with the quantities to be measured, x and y. Defining

$$\boldsymbol{\zeta} = (x\,y)^{\mathrm{T}}\,, \quad \boldsymbol{\mu_\zeta} = (\mu_x\,\mu_y)^{\mathrm{T}}\,, \quad \boldsymbol{b} = (b_x\,b_y)^{\mathrm{T}}\,, \quad \boldsymbol{\sigma} = \begin{pmatrix} \sigma_{xx} & \sigma_{xy} \\ \sigma_{yx} & \sigma_{yy} \end{pmatrix}\,,$$

we arrive at

$$z = \boldsymbol{b}^{\mathrm{T}}\boldsymbol{\zeta}\,, \quad \mu_z = E\{Z\} = \boldsymbol{b}^{\mathrm{T}}\boldsymbol{\mu_\zeta}\,, \quad \sigma_z^2 = E\left\{(Z-\mu_z)^2\right\} = \boldsymbol{b}^{\mathrm{T}}\boldsymbol{\sigma}\,\boldsymbol{b}\,.$$

We prove that Z is $N(\mu_z, \sigma_z^2)$ distributed. To this end we refer to the technique of characteristic functions. Given a random variable X, its characteristic function is defined by [43]

$$\chi(v) = E\left\{\mathrm{e}^{ivX}\right\} = \int_{-\infty}^{\infty} p_X(x)\mathrm{e}^{ivx}\,\mathrm{d}x\,. \tag{C.2}$$

If X is $N(\mu_x, \sigma_x^2)$ distributed, we have

$$\chi(v) = \exp\left(i\mu_x v - \frac{\sigma_x^2 v^2}{2}\right)\,. \tag{C.3}$$

Obviously, the Fourier transform of $\chi(v)$ reproduces the distribution density $p_X(x)$.

We consider the characteristic function of the random variable Z. Following (4.5) we may put

$$E\left\{\mathrm{e}^{ivZ}\right\} = \int_{-\infty}^{\infty} \mathrm{e}^{ivz} p_Z(z)\,\mathrm{d}z$$
$$= \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \exp\left[iv(b_x x + b_y y)\right] p\,(x,y)\,\mathrm{d}x\,\mathrm{d}y\,, \tag{C.4}$$

the density $p_{XY}(x,y)$ being given in (3.17),

$$p_{XY}(x,y) = \frac{1}{2\pi|\boldsymbol{\sigma}|^{1/2}} \exp\left[-\frac{1}{2}\left(\boldsymbol{\zeta}-\boldsymbol{\mu}_{\boldsymbol{\zeta}}\right)^{\mathrm{T}} \boldsymbol{\sigma}^{-1}\left(\boldsymbol{\zeta}-\boldsymbol{\mu}_{\boldsymbol{\zeta}}\right)\right].$$

Adding $\pm iv\boldsymbol{b}^{\mathrm{T}}\boldsymbol{\mu}_{\boldsymbol{\zeta}}$ to the exponent of (C.4), we form the identity

$$iv\,\boldsymbol{b}^{\mathrm{T}}\boldsymbol{\zeta} - \frac{1}{2}\left(\boldsymbol{\zeta}-\boldsymbol{\mu}_{\boldsymbol{\zeta}}\right)^{\mathrm{T}} \boldsymbol{\sigma}^{-1}\left(\boldsymbol{\zeta}-\boldsymbol{\mu}_{\boldsymbol{\zeta}}\right) \pm iv\,\boldsymbol{b}^{\mathrm{T}}\boldsymbol{\mu}_{\boldsymbol{\zeta}}$$
$$= -\frac{1}{2}\left(\boldsymbol{\zeta}-\boldsymbol{\mu}^{*}\right)^{\mathrm{T}} \boldsymbol{\sigma}^{-1}\left(\boldsymbol{\zeta}-\boldsymbol{\mu}^{*}\right) + iv\,\boldsymbol{b}^{\mathrm{T}}\boldsymbol{\mu}_{\boldsymbol{\zeta}} - \frac{v^2}{2}\,\boldsymbol{b}^{\mathrm{T}}\boldsymbol{\sigma}\,\boldsymbol{b}\,, \tag{C.5}$$

in which

$$\boldsymbol{\mu}^{*} = \boldsymbol{\mu}_{\boldsymbol{\zeta}} + iv\,vec\sigma\,.$$

Finally, (C.4) turns into

$$E\left\{\mathrm{e}^{ivZ}\right\} = \exp\left(i\boldsymbol{b}^{\mathrm{T}}\boldsymbol{\mu}_{\boldsymbol{\zeta}} v - \frac{\boldsymbol{b}^{\mathrm{T}}\boldsymbol{\sigma}\,\boldsymbol{b}v^2}{2}\right)$$
$$= \exp\left(i\mu_z v - \frac{\sigma_z^2\, v^2}{2}\right). \tag{C.6}$$

A comparison of (C.3) and (C.6) reveals that Z is normally distributed.

D Orthogonal Projections

Let $V_m(\Re)$ denote an m-dimensional vector space. Furthermore, let the $r < m$ linearly independent vectors

$$\boldsymbol{a}_1 = \begin{pmatrix} a_{11} \\ a_{21} \\ \cdots \\ a_{m1} \end{pmatrix}, \quad \boldsymbol{a}_2 = \begin{pmatrix} a_{12} \\ a_{22} \\ \cdots \\ a_{m2} \end{pmatrix}, \quad \ldots, \quad \boldsymbol{a}_r = \begin{pmatrix} a_{1r} \\ a_{2r} \\ \cdots \\ a_{mr} \end{pmatrix}$$

define an r-dimensional subspace $V_m^r(\Re) \subset V_m(\Re)$. We assemble the r vectors within a matrix

$$\boldsymbol{A} = (\boldsymbol{a}_1\, \boldsymbol{a}_2\, \cdots\, \boldsymbol{a}_r)$$

so that $V_m^r(\Re)$ coincides with the column space $R(\boldsymbol{A})$ of the matrix $\boldsymbol{A}$. The $(m-r)$-dimensional null space $N(\boldsymbol{A}^{\mathrm{T}}) = V_m^{m-r}(\Re)$ of the matrix $\boldsymbol{A}^{\mathrm{T}}$ is orthogonal to $R(\boldsymbol{A})$. The set of linear independent vectors $\boldsymbol{r}_1, \ldots, \boldsymbol{r}_{m-r}$, spanning $N(\boldsymbol{A}^{\mathrm{T}})$, is defined through the linear system

$$\boldsymbol{A}^{\mathrm{T}}\boldsymbol{r} = \boldsymbol{0}\,. \tag{D.1}$$

Each vector lying within $R(\boldsymbol{A})$ is orthogonal to each vector lying within $N(\boldsymbol{A}^{\mathrm{T}})$ and vice versa: $V_m(\Re)$ is the direct sum of the subspaces $R(\boldsymbol{A})$ and $N(\boldsymbol{A}^{\mathrm{T}})$,

$$V_m\left(\Re\right) = N\left(\boldsymbol{A}^{\mathrm{T}}\right) \oplus R\left(\boldsymbol{A}\right)\,.$$

Each vector $\boldsymbol{y}$ being an element of $R(\boldsymbol{A})$ may be uniquely decomposed into a linear combination of the vectors $\boldsymbol{a}_k$; $k = 1, \ldots, r$,

$$\boldsymbol{A}\boldsymbol{\beta} = \boldsymbol{y}\,. \tag{D.2}$$

The r components β_k; $k = 1, \ldots, r$ of the vector

$$\boldsymbol{\beta} = (\beta_1\, \beta_2\, \ldots\, \beta_r)^{\mathrm{T}}$$

may be seen as coefficients or "stretch factors" attributing to the vectors $\boldsymbol{a}_k$; $k = 1, \ldots, r$ suitable lengths so that the linear combination

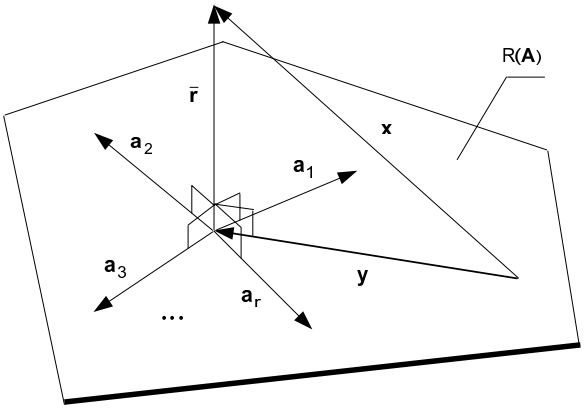


Fig. D.1. The r column vectors $\boldsymbol{a_1}, \boldsymbol{a_2}, \ldots, \boldsymbol{a_r}$ span an r-dimensional subspace $R(\boldsymbol{A}) = V_m^r(\Re)$ of the m-dimensional space $V_m(\Re)$. The vector of the residuals, $\bar{\boldsymbol{r}} \in N(\boldsymbol{A}^{\mathrm{T}})$, $N(\boldsymbol{A}^{\mathrm{T}}) \perp R(\boldsymbol{A})$, is orthogonal to the vectors $\boldsymbol{a_1}, \boldsymbol{a_2} \ldots, \boldsymbol{a_r}$

$$\beta_1 \boldsymbol{a}_1 + \beta_2 \boldsymbol{a}_2 + \cdots + \beta_r \boldsymbol{a}_r$$

defines, as desired, the vector $\boldsymbol{y}$.

Clearly, any vector $\boldsymbol{x} \in V_m(\Re)$ may only be represented through a linear combination of the vectors $\boldsymbol{a}_k$; $k = 1, \ldots, r$ if it happens that $\boldsymbol{x}$ lies in $R(\boldsymbol{A}) \subset V_m(\Re)$. This, however, will in general not be the case. In view of Fig. D.1 we consider the orthogonal projection of $\boldsymbol{x}$ onto $R(\boldsymbol{A})$.[1]

Let $\boldsymbol{P}$ be an operator accomplishing the orthogonal projection of $\boldsymbol{x}$ onto $R(\boldsymbol{A})$,

$$\boldsymbol{y} = \boldsymbol{P}\boldsymbol{x} = \boldsymbol{A}\boldsymbol{\beta}\,. \tag{D.3}$$

We shall show that the column vectors $\boldsymbol{a}_k$; $k = 1, \ldots, r$ of the matrix $\boldsymbol{A}$ determine the structure of the projection operator $\boldsymbol{P}$. Let $\bar{\boldsymbol{r}} \in N(\boldsymbol{A}^{\mathrm{T}})$ denote the component of $\boldsymbol{x}$ perpendicular to $R(\boldsymbol{A}) = V_m^r(\Re)$. We then have

$$\bar{\boldsymbol{r}} = \boldsymbol{x} - \boldsymbol{y}\,; \quad \boldsymbol{A}^{\mathrm{T}}\bar{\boldsymbol{r}} = \boldsymbol{0}\,. \tag{D.4}$$

Any linear combination of the $m-r$ linearly independent vectors spanning the null space $N(\boldsymbol{A}^{\mathrm{T}}) = V_m^{m-r}(\Re)$ of the matrix $\boldsymbol{A}^{\mathrm{T}}$ is orthogonal to the vectors $\boldsymbol{a}_k$; $k = 1, \ldots, r$ spanning the column space $R(\boldsymbol{A}) = V_m^r(\Re)$. However, given $\boldsymbol{P}$, the orthogonal projection $\boldsymbol{y} = \boldsymbol{P}\boldsymbol{x}$ of $\boldsymbol{x}$ onto $R(\boldsymbol{A})$ is fixed. At the same time, out of all vectors $\boldsymbol{r}$ satisfying $\boldsymbol{A}^{\mathrm{T}}\boldsymbol{r} = \boldsymbol{0}$, the vector of the residuals $\bar{\boldsymbol{r}} = \boldsymbol{x} - \boldsymbol{P}\boldsymbol{x}$ is selected.

Suppose we had an orthonormal basis

[1] Should $\boldsymbol{x}$ already lie in $R(\boldsymbol{A})$, the projection would not entail any change at all.

$$\boldsymbol{\alpha}_1 = \begin{pmatrix} \alpha_{11} \\ \alpha_{21} \\ \cdots \\ \alpha_{m1} \end{pmatrix}, \quad \ldots, \quad \boldsymbol{\alpha}_m = \begin{pmatrix} \alpha_{1m} \\ \alpha_{2m} \\ \cdots \\ \alpha_{mm} \end{pmatrix}$$

of the space $V_m(\Re)$. Let the first r vectors define the column space $R(\boldsymbol{A})$ and let the last $m-r$ span the null space $N(\boldsymbol{A}^{\mathrm{T}})$. Thus, for any vector $\boldsymbol{x} \in V_m(\Re)$ we have

$$\begin{aligned} \boldsymbol{x} &= \underbrace{\gamma_1\boldsymbol{\alpha}_1 + \cdots + \gamma_r\boldsymbol{\alpha}_r}_{\boldsymbol{y}} \quad + \quad \underbrace{\gamma_{r+1}\boldsymbol{\alpha}_{r+1} + \cdots + \gamma_m\boldsymbol{\alpha}_m}_{\bar{\boldsymbol{r}}}; \\ \boldsymbol{\alpha}_k^{\mathrm{T}}\boldsymbol{x} &= \gamma_k\,; \quad k = 1, \ldots, m\,, \end{aligned} \tag{D.5}$$

or

$$\boldsymbol{y} = \sum_{k=1}^{r} \gamma_k\boldsymbol{\alpha}_k\,, \quad \bar{\boldsymbol{r}} = \sum_{k=r+1}^{m} \gamma_k\boldsymbol{\alpha}_k\,.$$

By means of the first r vectors $\boldsymbol{\alpha}_k$; $k = 1, \ldots, r$ we define a matrix

$$\boldsymbol{T} = \begin{pmatrix} \alpha_{11} & \alpha_{12} & \ldots & \alpha_{1r} \\ \alpha_{21} & \alpha_{22} & \ldots & \alpha_{2r} \\ \cdots & \cdots & \cdots & \cdots \\ \alpha_{m1} & \alpha_{m2} & \ldots & \alpha_{mr} \end{pmatrix}\,; \quad \boldsymbol{T}^{\mathrm{T}}\boldsymbol{T} = \boldsymbol{I}\,. \tag{D.6}$$

Here, $\boldsymbol{I}$ designates an $(r \times r)$ identity matrix. In contrast to this, the product $\boldsymbol{T}\,\boldsymbol{T}^{\mathrm{T}}$ accomplishes the desired orthogonal projection, since from

$$(\gamma_1\,\gamma_2\,\cdots\,\gamma_r)^{\mathrm{T}} = \boldsymbol{T}^{\mathrm{T}}\boldsymbol{x}$$

we find

$$\boldsymbol{y} = \boldsymbol{T}\,(\gamma_1\,\gamma_2\,\cdots\,\gamma_r)^{\mathrm{T}} = \boldsymbol{T}\,\boldsymbol{T}^{\mathrm{T}}\boldsymbol{x} = \boldsymbol{P}\boldsymbol{x}\,, \quad \boldsymbol{P} = \boldsymbol{T}\,\boldsymbol{T}^{\mathrm{T}}\,. \tag{D.7}$$

The projection operator $\boldsymbol{P}$ has now been established. But this has been done with reference to an orthogonal basis, which actually we do not possess. In order to express $\boldsymbol{P}$ by means of the vectors $\boldsymbol{a}_k$; $k = 1, \ldots, r$ of the column space of $\boldsymbol{A}$, we define a non-singular $(r \times r)$ auxiliary matrix $\boldsymbol{H}$ so that

$$\boldsymbol{A} = \boldsymbol{T}\,\boldsymbol{H}\,. \tag{D.8}$$

Following (D.6) we have $\boldsymbol{H} = \boldsymbol{T}^{\mathrm{T}}\boldsymbol{A}$ and, furthermore, $\boldsymbol{T} = \boldsymbol{A}\boldsymbol{H}^{-1}$, i.e.

$$\boldsymbol{P} = \boldsymbol{T}\,\boldsymbol{T}^{\mathrm{T}} = \boldsymbol{A}\boldsymbol{H}^{-1}\left(\boldsymbol{H}^{-1}\right)^{\mathrm{T}}\boldsymbol{A}^{\mathrm{T}} = \boldsymbol{A}\left(\boldsymbol{H}^{\mathrm{T}}\boldsymbol{H}\right)^{-1}\boldsymbol{A}^{\mathrm{T}}\,,$$

and as

$$\boldsymbol{H}^{\mathrm{T}}\boldsymbol{H} = \boldsymbol{A}^{\mathrm{T}}\boldsymbol{T}\boldsymbol{T}^{\mathrm{T}}\boldsymbol{A} = \boldsymbol{A}^{\mathrm{T}}\boldsymbol{P}\boldsymbol{A} = \boldsymbol{A}^{\mathrm{T}}\boldsymbol{A}\,,$$

$\boldsymbol{P}\boldsymbol{A} = \boldsymbol{A}$, we finally arrive at

$$\boldsymbol{P} = \boldsymbol{A}\left(\boldsymbol{A}^{\mathrm{T}}\boldsymbol{A}\right)^{-1}\boldsymbol{A}^{\mathrm{T}}\,. \tag{D.9}$$

This operator, expressed in terms of $\boldsymbol{A}$, accomplishes the desired orthogonal projection of $\boldsymbol{x}$ onto $R(\boldsymbol{A})$.

Should there be two different projection operators $\boldsymbol{P}_1\boldsymbol{x} = \boldsymbol{y}$, $\boldsymbol{P}_2\boldsymbol{x} = \boldsymbol{y}$, we necessarily have

$$(\boldsymbol{P}_1 - \boldsymbol{P}_2)\,\boldsymbol{x} = \boldsymbol{0}$$

which is not, however, possible for arbitrary vectors $\boldsymbol{x}$. From this we conclude that projection operators are unique.

We easily convince ourselves once again that the projection of any vector lying already within $R(\boldsymbol{A})$ simply reproduces just this vector. Indeed, from (D.7) we obtain

$$\boldsymbol{P}\boldsymbol{y} = \boldsymbol{T}\,\boldsymbol{T}^{\mathrm{T}}\boldsymbol{T}\,(\gamma_1\,\gamma_2\,\cdots\,\gamma_r)^{\mathrm{T}} = \boldsymbol{T}\,(\gamma_1\,\gamma_2\,\cdots\,\gamma_r)^{\mathrm{T}} = \boldsymbol{y}\,.$$

Projection operators possess the property $\boldsymbol{P}^2 = \boldsymbol{P}$, i.e. they are idempotent. Furthermore, they are symmetric. Vice versa, any symmetric matrix showing $\boldsymbol{P}^2 = \boldsymbol{P}$ is a projection operator.

As rank $(\boldsymbol{A}) = r$, we have rank $(\boldsymbol{P}) = r$. Let $\boldsymbol{v}$ be an eigenvector of $\boldsymbol{P}$ and $\lambda \neq 0$ the pertaining eigenvalue, $\boldsymbol{P}\boldsymbol{v} = \lambda v$. Then from $\boldsymbol{P}(\boldsymbol{P}\boldsymbol{v}) = \lambda^2\boldsymbol{v} = \boldsymbol{P}\boldsymbol{v} = \lambda v$, i.e. $\lambda^2 = \lambda$, we see $\lambda = 1$. The eigenvalues of projection operators are either 0 or 1.

Obviously, the trace of $\boldsymbol{P}$ is given by the sum of its eigenvalues, at the same time the rank of an indempotent matrix equals its trace. From this we conclude that r eigenvalues are 1 and $m - r$ eigenvalues are 0 [52–54].

E Least Squares Adjustments

We refer to the nomenclature of Appendix D.

Unconstrained Adjustment

The linear system

$$\boldsymbol{A\beta} \approx \boldsymbol{x} \tag{E.1}$$

is unsolvable as, due to the measurement errors, $\boldsymbol{x} \in V_m(\Re)$ and $\boldsymbol{A\beta} \in V_m^r(\Re)$, where least squares presupposes $r < m$. Let us decompose $V_m(\Re)$ into orthogonal subspaces $V_m^r(\Re)$ and $V_m^{m-r}(\Re)$ so that

$$V_m\left(\Re\right) = V_m^r\left(\Re\right) \oplus V_m^{m-r}\left(\Re\right) .$$

The method of least squares projects the vector $\boldsymbol{x}$ by means of the projection operator

$$\boldsymbol{P} = \boldsymbol{A}\left(\boldsymbol{A}^{\mathrm{T}}\boldsymbol{A}\right)^{-1}\boldsymbol{A}^{\mathrm{T}} \tag{E.2}$$

orthogonally onto the subspace $V_m^r(\Re)$, so that $\boldsymbol{Px} \in V_m^r(\Re)$. The orthogonal projection defines a so-called vector of residuals $\bar{\boldsymbol{r}}$ satisfying $\boldsymbol{A^T}\bar{\boldsymbol{r}} = \boldsymbol{0}$, $\bar{\boldsymbol{r}} \in V_m^{m-r}(\Re)$ and $\boldsymbol{x} - \bar{\boldsymbol{r}} = \boldsymbol{Px} \in V_m^r(\Re)$.[1] Ignoring $\bar{\boldsymbol{r}}$ and substituting the vector $\boldsymbol{Px}$ for $\boldsymbol{x}$,

$$\boldsymbol{A}\bar{\boldsymbol{\beta}} = \boldsymbol{Px}\,, \tag{E.3}$$

the inconsistent system (E.1) becomes "solvable". After all, the quintessence of the method of least squares is rooted in this substitution, which is, frankly speaking, a trick. Multiplying (E.3) on the left by $(\boldsymbol{A}^{\mathrm{T}}\boldsymbol{A})^{-1}\boldsymbol{A}^{\mathrm{T}}$ yields the least squares estimator

$$\bar{\boldsymbol{\beta}} = \left(\boldsymbol{A}^{\mathrm{T}}\boldsymbol{A}\right)^{-1}\boldsymbol{A}^{\mathrm{T}}\boldsymbol{x} \tag{E.4}$$

of the unknown true solution vector.

[1] There are, of course, infinitely many vectors $\boldsymbol{r} \in V_m^{m-r}(\Re)$ satisfying $\boldsymbol{A}^{\mathrm{T}}\boldsymbol{r} = \boldsymbol{0}$. The orthogonal projection through $\boldsymbol{P}$ selects the vector of residuals $\bar{\boldsymbol{r}}$.

Constrained Adjustment

1. rank $(\boldsymbol{A}) = r$

The least squares estimator $\bar{\boldsymbol{\beta}}$ shall exactly satisfy $q < r$ constraints

$$\boldsymbol{H}\bar{\boldsymbol{\beta}} = \boldsymbol{y}\,, \tag{E.5}$$

where rank $(\boldsymbol{H}) = q$ is assumed. Although we adhere to the idea of orthogonal projection, we of course have to alter the projection operator, i.e. though we require the new $\boldsymbol{P}$ to accomplish $\boldsymbol{P}\boldsymbol{x} \in V_m^r(\Re)$, this new $\boldsymbol{P}$ will be different from the projection operator of the unconstrained adjustment.

First, we introduce an auxiliary vector $\boldsymbol{\beta}^*$ leading to homogeneous constraints – later on this vector will cancel.

Let $\boldsymbol{\beta}^*$ be any solution of the linear constraints (E.5),

$$\boldsymbol{H}\boldsymbol{\beta}^* = \boldsymbol{y}\,. \tag{E.6}$$

Then, from

$$\boldsymbol{A}\,(\boldsymbol{\beta} - \boldsymbol{\beta}^*) \approx \boldsymbol{x} - \boldsymbol{A}\boldsymbol{\beta}^*\,, \quad \boldsymbol{H}\,(\boldsymbol{\beta} - \boldsymbol{\beta}^*) = \boldsymbol{0}$$

we obtain, setting

$$\boldsymbol{\gamma} = \boldsymbol{\beta} - \boldsymbol{\beta}^*\,, \quad \boldsymbol{z} = \boldsymbol{x} - \boldsymbol{A}\boldsymbol{\beta}^*\,, \tag{E.7}$$

the new systems

$$\boldsymbol{A}\boldsymbol{\gamma} \approx \boldsymbol{z}\,, \quad \boldsymbol{H}\boldsymbol{\gamma} = \boldsymbol{0}\,. \tag{E.8}$$

Let us assume that the new projection operator $\boldsymbol{P}$ is known. Hence, $\boldsymbol{P}$ projects $\boldsymbol{z}$ orthogonally onto the column space of $\boldsymbol{A}$,

$$\boldsymbol{A}\bar{\boldsymbol{\gamma}} = \boldsymbol{P}\boldsymbol{z}\,, \quad \boldsymbol{P} \neq \boldsymbol{A}\left(\boldsymbol{A}^{\mathrm{T}}\boldsymbol{A}\right)^{-1}\boldsymbol{A}^{\mathrm{T}} \quad \text{here} \tag{E.9}$$

so that

$$\bar{\boldsymbol{\gamma}} = \left(\boldsymbol{A}^{\mathrm{T}}\boldsymbol{A}\right)^{-1}\boldsymbol{A}^{\mathrm{T}}\boldsymbol{P}\boldsymbol{z}\,. \tag{E.10}$$

Obviously, the condition

$$\boldsymbol{H}\bar{\boldsymbol{\gamma}} = \boldsymbol{H}\left(\boldsymbol{A}^{\mathrm{T}}\boldsymbol{A}\right)^{-1}\boldsymbol{A}^{\mathrm{T}}\boldsymbol{P}\boldsymbol{z} = \boldsymbol{C}^{\mathrm{T}}\boldsymbol{P}\boldsymbol{z} = \boldsymbol{0} \tag{E.11}$$

is fulfilled, given the vector $\boldsymbol{P}\boldsymbol{z}$ lies in the null space of the matrix

$$\boldsymbol{C}^{\mathrm{T}} = \boldsymbol{H}\left(\boldsymbol{A}^{\mathrm{T}}\boldsymbol{A}\right)^{-1}\boldsymbol{A}^{\mathrm{T}}\,.$$

Finally, $\boldsymbol{P}\boldsymbol{z}$ has to lie in the column space of the matrix $\boldsymbol{A}$ as well as in the null space of the matrix $\boldsymbol{C}^{\mathrm{T}}$, i.e.

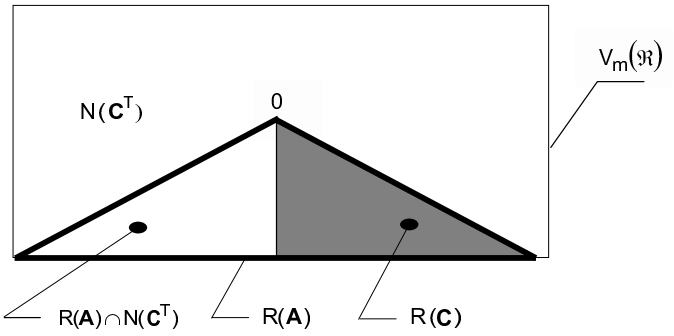


Fig. E.1. $V_m^r(\Re)$ symbolic, $R(\boldsymbol{C}) \subset R(\boldsymbol{A})$, $R(\boldsymbol{C}) \perp N(\boldsymbol{C}^{\mathbf{T}})$, intersection $R(\boldsymbol{A}) \cap N(\boldsymbol{C}^{\mathrm{T}})$

$$\boldsymbol{P}\boldsymbol{z} \in R\left(\boldsymbol{A}\right) \cap N\left(\boldsymbol{C}^{\mathrm{T}}\right) .$$

The q linearly independent column vectors of the matrix $\boldsymbol{C}$ span a q-dimensional subspace $R(\boldsymbol{C}) = V_m^q(\Re)$ of the space $R(\boldsymbol{A}) = V_m^r(\Re)$, where $R(\boldsymbol{C}) \subset R(\boldsymbol{A})$. Furthermore, as

$$N(\boldsymbol{C}^{\mathrm{T}}) = V_m^{m-q}\left(\Re\right) , \quad R\left(\boldsymbol{C}\right) \perp N(\boldsymbol{C}^{\mathrm{T}}) \quad \text{and} \quad R\left(\boldsymbol{C}\right) \oplus N(\boldsymbol{C}^{\mathrm{T}}) = V_m\left(\Re\right) ,$$

the intersection $R(\boldsymbol{A}) \cap N(\boldsymbol{C}^{\mathrm{T}})$ is well defined, Fig. E.1. To project in just this intersection, we simply put

$$\boldsymbol{P} = \boldsymbol{A}\left(\boldsymbol{A}^{\mathrm{T}}\boldsymbol{A}\right)^{-1}\boldsymbol{A}^{\mathrm{T}} - \boldsymbol{C}\left(\boldsymbol{C}^{\mathrm{T}}\boldsymbol{C}\right)^{-1}\boldsymbol{C}^{\mathrm{T}}$$

so that the component projected onto $R(\boldsymbol{C})$, $R(\boldsymbol{C}) \subset R(\boldsymbol{A})$ cancels. Returning to $\bar{\boldsymbol{\beta}}$ yields

$$\begin{aligned} \bar{\boldsymbol{\beta}} &= \left(\boldsymbol{A}^{\mathrm{T}}\boldsymbol{A}\right)^{-1}\boldsymbol{A}^{\mathrm{T}}\boldsymbol{x} \\ &\quad - \left(\boldsymbol{A}^{\mathrm{T}}\boldsymbol{A}\right)^{-1}\boldsymbol{H}^{\mathrm{T}}\left[\boldsymbol{H}\left(\boldsymbol{A}^{\mathrm{T}}\boldsymbol{A}\right)^{-1}\boldsymbol{H}^{\mathrm{T}}\right]^{-1}\left[\boldsymbol{H}\left(\boldsymbol{A}^{\mathrm{T}}\boldsymbol{A}\right)^{-1}\boldsymbol{A}^{\mathrm{T}}\boldsymbol{x} - \boldsymbol{y}\right] . \end{aligned} \tag{E.12}$$

Finally, we see $\boldsymbol{H}\bar{\boldsymbol{\beta}} = \boldsymbol{y}$.

2. rank $(\boldsymbol{A}) = r' < r$

We assume the first r' column vectors of the matrix $\boldsymbol{A}$ to be linearly independent. Then, we partition the matrix $\boldsymbol{A}$ into an $(m \times r')$ matrix $\boldsymbol{A}_1$ and an $(m \times (r - r'))$ matrix $\boldsymbol{A}_2$,

$$\boldsymbol{A} = \left(\boldsymbol{A}_1 \,|\, \boldsymbol{A}_2\right) .$$

Formally, the inconsistencies of the system (E.1) "vanish", when the erroneous vector $\boldsymbol{x}$ is projected onto the column space of $\boldsymbol{A}_1$,

$$\boldsymbol{A}\bar{\boldsymbol{\beta}} = \boldsymbol{P}\boldsymbol{x}\,, \quad \boldsymbol{P} = \boldsymbol{A}_1 \left(\boldsymbol{A}_1^{\mathrm{T}}\boldsymbol{A}_1\right)^{-1} \boldsymbol{A}_1^{\mathrm{T}}\,. \tag{E.13}$$

However, as rank $(\boldsymbol{A}) = r' < r$, there are $q = (r - r')$ indeterminate components of the vector $\bar{\boldsymbol{\beta}}$. Consequently, we may add q constraints. As the column vectors $\boldsymbol{a}_k$; $k = r' + 1, \ldots, r$ are linear combinations of the column vectors $\boldsymbol{a}_k$; $k = 1, \ldots, r'$ and the projection of any vector lying in the column space of $\boldsymbol{A}_1$ simply gets reproduced, we have $\boldsymbol{P}\boldsymbol{A} = \boldsymbol{A}$ or $(\boldsymbol{P}\boldsymbol{A})^{\mathrm{T}} = \boldsymbol{A}^{\mathrm{T}}\boldsymbol{P} = \boldsymbol{A}^{\mathrm{T}}$. Hence, multiplying (E.13) on the left by $\boldsymbol{A}^{\mathrm{T}}$ yields

$$\boldsymbol{A}^{\mathrm{T}}\boldsymbol{A}\bar{\boldsymbol{\beta}} = \boldsymbol{A}^{\mathrm{T}}\boldsymbol{x}\,. \tag{E.14}$$

Adding $q = r - r'$ constraints, we may solve the two systems simultaneously. To this end, we multiply (E.5) on left by $\boldsymbol{H}^{\mathrm{T}}$,

$$\boldsymbol{H}^{\mathrm{T}}\boldsymbol{H}\bar{\boldsymbol{\beta}} = \boldsymbol{H}^{\mathrm{T}}\boldsymbol{y}\,, \tag{E.15}$$

so that

$$\left(\boldsymbol{A}^{\mathrm{T}}\boldsymbol{A} + \boldsymbol{H}^{\mathrm{T}}\boldsymbol{H}\right)\bar{\boldsymbol{\beta}} = \boldsymbol{A}^{\mathrm{T}}\boldsymbol{x} + \boldsymbol{H}^{\mathrm{T}}\boldsymbol{y}\,. \tag{E.16}$$

Obviously, the auxiliary matrix

$$\boldsymbol{C} = \begin{pmatrix} \boldsymbol{A} \\ -- \\ \boldsymbol{H} \end{pmatrix}$$

possesses r' linearly independent rows in $\boldsymbol{A}$ and $q = r - r'$ linearly independent rows in $\boldsymbol{H}$ so that rank $(\boldsymbol{C}) = r$. But then, the product matrix

$$\boldsymbol{C}^{\mathrm{T}}\boldsymbol{C} = \left(\boldsymbol{A}^{\boldsymbol{T}}\boldsymbol{A} + \boldsymbol{H}^{\boldsymbol{T}}\boldsymbol{H}\right)$$

has the same rank. Finally, (E.16) yields

$$\bar{\boldsymbol{\beta}} = \left(\boldsymbol{A}^{\mathrm{T}}\boldsymbol{A} + \boldsymbol{H}^{\mathrm{T}}\boldsymbol{H}\right)^{-1} \left(\boldsymbol{A}^{\mathrm{T}}\boldsymbol{x} + \boldsymbol{H}^{\mathrm{T}}\boldsymbol{y}\right)\,. \tag{E.17}$$

The two relationships [8],

$$\boldsymbol{H}\left(\boldsymbol{A}^{\mathrm{T}}\boldsymbol{A} + \boldsymbol{H}^{\mathrm{T}}\boldsymbol{H}\right)^{-1}\boldsymbol{A}^{\mathrm{T}} = \boldsymbol{0} \quad \text{and} \quad \boldsymbol{H}\left(\boldsymbol{A}^{\mathrm{T}}\boldsymbol{A} + \boldsymbol{H}^{\mathrm{T}}\boldsymbol{H}\right)^{-1}\boldsymbol{H}^{\mathrm{T}} = \boldsymbol{I}\,,$$

where $\boldsymbol{I}$ denotes a $(q \times q)$ identity matrix, disclose that $\bar{\boldsymbol{\beta}}$ satisfies $\boldsymbol{H}\bar{\boldsymbol{\beta}} = \boldsymbol{y}$.

F Expansion of Solution Vectors

Section 11.1: Planes

The design matrix

$$\boldsymbol{A} = \begin{pmatrix} 1 & \bar{x}_1 & \bar{y}_1 \\ 1 & \bar{x}_2 & \bar{y}_2 \\ \cdots & \cdots & \cdots \\ 1 & \bar{x}_m & \bar{y}_m \end{pmatrix}$$

leads us to the product

$$\boldsymbol{A}^{\mathrm{T}}\boldsymbol{A} = \begin{pmatrix} H_{11} & H_{12} & H_{13} \\ H_{21} & H_{22} & H_{23} \\ H_{31} & H_{32} & H_{33} \end{pmatrix}$$

in which

$$H_{11} = m\,, \qquad H_{22} = \sum_{j=1}^{m} \bar{x}_j^2\,, \qquad H_{33} = \sum_{j=1}^{m} \bar{y}_j^2$$

$$H_{12} = H_{21} = \sum_{j=1}^{m} \bar{x}_j\,, \quad H_{13} = H_{31} = \sum_{j=1}^{m} \bar{y}_j\,, \quad H_{23} = H_{32} = \sum_{j=1}^{m} \bar{x}_j \bar{y}_j\,.$$

Let D denote the determinant of $\boldsymbol{A}^{\mathrm{T}}\boldsymbol{A}$,

$$\begin{aligned} D = {} & H_{11}\left(H_{22}H_{33} - H_{23}^2\right) + H_{12}\left(H_{31}H_{23} - H_{33}H_{12}\right) \\ & + H_{13}\left(H_{21}H_{32} - H_{13}H_{22}\right)\,. \end{aligned}$$

Obviously,

$$\left(\boldsymbol{A}^{\mathrm{T}}\boldsymbol{A}\right)^{-1} = \frac{1}{D}\begin{pmatrix} H_{22}H_{33} - H_{23}^2 & \mid H_{23}H_{13} - H_{12}H_{33} & \mid H_{12}H_{23} - H_{22}H_{13} \\ H_{23}H_{13} - H_{12}H_{33} & \mid H_{11}H_{33} - H_{13}^2 & \mid H_{12}H_{13} - H_{11}H_{23} \\ H_{12}H_{23} - H_{22}H_{13} & \mid H_{12}H_{13} - H_{11}H_{23} & \mid H_{11}H_{22} - H_{12}^2 \end{pmatrix}$$

is the inverse of $\boldsymbol{A}^{\mathrm{T}}\boldsymbol{A}$. Putting $\boldsymbol{B} = \boldsymbol{A}\left(\boldsymbol{A}^{\mathrm{T}}\boldsymbol{A}\right)^{-1}$, the components of $\bar{\boldsymbol{\beta}} = \boldsymbol{B}^{\mathrm{T}}\bar{\boldsymbol{z}}$ are given by

$$\bar{\beta}_1 = \sum_{j=1}^{m} b_{j1}\bar{z}_j\,, \quad \bar{\beta}_2 = \sum_{j=1}^{m} b_{j2}\bar{z}_j\,, \quad \bar{\beta}_3 = \sum_{j=1}^{m} b_{j3}\bar{z}_j$$

or

$$\begin{aligned}
\bar{\beta}_1 &= \frac{1}{D}\sum_{j=1}^{m}\left\{\left[H_{22}H_{33} - H_{23}^2\right] + \left[H_{23}H_{13} - H_{12}H_{33}\right]\bar{x}_j\right.\\
&\quad \left. + \left[H_{12}H_{23} - H_{22}H_{13}\right]\bar{y}_j\right\}\bar{z}_j\\
\bar{\beta}_2 &= \frac{1}{D}\sum_{j=1}^{m}\left\{\left[H_{23}H_{13} - H_{12}H_{33}\right] + \left[H_{11}H_{33} - H_{13}^2\right]\bar{x}_j\right.\\
&\quad \left. + \left[H_{12}H_{13} - H_{11}H_{23}\right]\bar{y}_j\right\}\bar{z}_j\\
\bar{\beta}_3 &= \frac{1}{D}\sum_{j=1}^{m}\left\{\left[H_{12}H_{23} - H_{22}H_{13}\right] + \left[H_{12}H_{13} - H_{11}H_{23}\right]\bar{x}_j\right.\\
&\quad \left. + \left[H_{11}H_{22} - H_{12}^2\right]\bar{y}_j\right\}\bar{z}_j\,.
\end{aligned}$$

Before writing down the partial derivatives, we differentiate the determinant,

$$\begin{aligned}
\frac{\partial D}{\partial \bar{x}_i} &= 2\left[H_{11}H_{33} - H_{13}^2\right]\bar{x}_i + 2\left[H_{12}H_{13} - H_{11}H_{23}\right]\bar{y}_i\\
&\quad +2\left[H_{13}H_{23} - H_{12}H_{33}\right]\\
\frac{\partial D}{\partial \bar{y}_i} &= 2\left[H_{12}H_{13} - H_{11}H_{23}\right]\bar{x}_i + 2\left[H_{11}H_{22} - H_{12}^2\right]\bar{y}_i\\
&\quad +2\left[H_{12}H_{23} - H_{13}H_{22}\right]\\
\frac{\partial D}{\partial \bar{z}_i} &= 0\,.
\end{aligned}$$

Now, each of the components $\bar{\beta}_k$; $k = 1, 2, 3$ has to be partially differentiated with respect to x, y and z,

$$\begin{aligned}
c_{i1} = \frac{\partial \bar{\beta}_1}{\partial \bar{x}_i} &= -\frac{\bar{\beta}_1}{D}\frac{\partial D}{\partial \bar{x}_i}\\
&\quad +\frac{1}{D}\left\{2\left(H_{33}\bar{x}_i - H_{23}\bar{y}_i\right)\sum_{j=1}^{m}\bar{z}_j + \left(H_{13}H_{23} - H_{12}H_{33}\right)\bar{z}_i\right.\\
&\quad \left. + \left(H_{13}\bar{y}_i - H_{33}\right)\sum_{j=1}^{m}\bar{x}_j\bar{z}_j + \left(H_{23} + H_{12}\bar{y}_i - 2H_{13}\bar{x}_i\right)\sum_{j=1}^{m}\bar{y}_j\bar{z}_j\right\}
\end{aligned}$$

$$
\begin{aligned}
c_{i+m,1} &= \frac{\partial \bar{\beta}_1}{\partial \bar{y}_i} = -\frac{\bar{\beta}_1}{D}\frac{\partial D}{\partial \bar{y}_i} \\
&\quad + \frac{1}{D}\left\{ 2\left(H_{22}\bar{y}_i - H_{23}\bar{x}_i\right)\sum_{j=1}^{m}\bar{z}_j + \left(H_{12}H_{23} - H_{13}H_{22}\right)\bar{z}_i \right. \\
&\quad \left. + \left(H_{23} + H_{13}\bar{x}_i - 2H_{12}\bar{y}_i\right)\sum_{j=1}^{m}\bar{x}_j\bar{z}_j + \left(H_{12}\bar{x}_i - H_{22}\right)\sum_{j=1}^{m}\bar{y}_j\bar{z}_j \right\} \\
c_{i+2m,1} &= \frac{\partial \bar{\beta}_1}{\partial \bar{z}_i} = b_{i1} \\
c_{i2} &= \frac{\partial \bar{\beta}_2}{\partial \bar{x}_i} = -\frac{\bar{\beta}_2}{D}\frac{\partial D}{\partial \bar{x}_i} + \frac{1}{D}\left\{ \left(H_{13}\bar{y}_i - H_{33}\right)\sum_{j=1}^{m}\bar{z}_j \right. \\
&\quad \left. + \left(H_{11}H_{33} - H_{13}^2\right)\bar{z}_i + \left(H_{13} - H_{11}\bar{y}_i\right)\sum_{j=1}^{m}\bar{y}_j\bar{z}_j \right\} \\
c_{i+m,2} &= \frac{\partial \bar{\beta}_2}{\partial \bar{y}_i} = -\frac{\bar{\beta}_2}{D}\frac{\partial D}{\partial \bar{y}_i} + \frac{1}{D}\left\{ \left(H_{23} + H_{13}\bar{x}_i - 2H_{12}\bar{y}_i\right)\sum_{j=1}^{m}\bar{z}_j \right. \\
&\quad + \left(H_{12}H_{13} - H_{11}H_{23}\right)\bar{z}_i + 2\left(H_{11}\bar{y}_i - H_{13}\right)\sum_{j=1}^{m}\bar{x}_j\bar{z}_j \\
&\quad \left. + \left(H_{12} - H_{11}\bar{x}_i\right)\sum_{j=1}^{m}\bar{y}_j\bar{z}_j \right\} \\
c_{i+2m,2} &= \frac{\partial \bar{\beta}_2}{\partial \bar{z}_i} = b_{i2} \\
c_{i3} &= \frac{\partial \bar{\beta}_3}{\partial \bar{x}_i} = -\frac{\bar{\beta}_3}{D}\frac{\partial D}{\partial \bar{x}_i} + \frac{1}{D}\left\{ \left(H_{23} + H_{12}\bar{y}_i - 2H_{13}\bar{x}_i\right)\sum_{j=1}^{m}\bar{z}_j \right. \\
&\quad + \left(H_{12}H_{13} - H_{11}H_{23}\right)\bar{z}_i \\
&\quad \left. + \left(H_{13} - H_{11}\bar{y}_i\right)\sum_{j=1}^{m}\bar{x}_j\bar{z}_j + 2\left(H_{11}\bar{x}_i - H_{12}\right)\sum_{j=1}^{m}\bar{y}_j\bar{z}_j \right\} \\
c_{i+m,3} &= \frac{\partial \bar{\beta}_3}{\partial \bar{y}_i} = -\frac{\bar{\beta}_3}{D}\frac{\partial D}{\partial \bar{y}_i} + \frac{1}{D}\left\{ \left(H_{12}\bar{x}_i - H_{22}\right)\sum_{j=1}^{m}\bar{z}_j \right. \\
&\quad \left. + \left(H_{11}H_{22} - H_{12}^2\right)\bar{z}_i + \left(H_{12} - H_{11}\bar{x}_i\right)\sum_{j=1}^{m}\bar{x}_j\bar{z}_j \right\}
\end{aligned}
$$

$$c_{i+2m,3} = \frac{\partial \bar{\beta}_3}{\partial \bar{z}_i} = b_{i3}\,.$$

Section 11.1: Parabolas

From the design matrix

$$\boldsymbol{A} = \begin{pmatrix} 1 & \bar{x}_1 & \bar{x}_1^2 \\ 1 & \bar{x}_2 & \bar{x}_2^2 \\ \cdots & \cdots & \cdots \\ 1 & \bar{x}_m & \bar{x}_m^2 \end{pmatrix}$$

we find the product matrix

$$\boldsymbol{A}^{\mathrm{T}}\boldsymbol{A} = \begin{pmatrix} H_{11} & H_{12} & H_{13} \\ H_{21} & H_{22} & H_{23} \\ H_{31} & H_{32} & H_{33} \end{pmatrix}$$

whose elements are given by

$$H_{11} = m\,, \qquad H_{22} = \sum_{j=1}^{m} \bar{x}_j^2\,, \qquad H_{33} = \sum_{j=1}^{m} \bar{x}_j^4$$

$$H_{12} = H_{21} = \sum_{j=1}^{m} \bar{x}_j\,, \quad H_{13} = H_{31} = \sum_{j=1}^{m} \bar{x}_j^2\,, \quad H_{23} = H_{32} = \sum_{j=1}^{m} \bar{x}_j^3\,.$$

Designating the determinant of $\boldsymbol{A}^{\mathrm{T}}\boldsymbol{A}$ by

$$\begin{aligned} D = {} & H_{11}\left(H_{22}H_{33} - H_{23}^2\right) + H_{12}\left(H_{31}H_{23} - H_{33}H_{12}\right) \\ & + H_{13}\left(H_{21}H_{32} - H_{13}H_{22}\right)\,. \end{aligned}$$

we find

$$\left(\boldsymbol{A}^{\mathrm{T}}\boldsymbol{A}\right)^{-1} = \frac{1}{D}\begin{pmatrix} H_{22}H_{33} - H_{23}^2 & | & H_{23}H_{13} - H_{12}H_{33} & | & H_{12}H_{23} - H_{22}H_{13} \\ H_{23}H_{13} - H_{12}H_{33} & | & H_{11}H_{33} - H_{13}^2 & | & H_{12}H_{13} - H_{11}H_{23} \\ H_{12}H_{23} - H_{22}H_{13} & | & H_{12}H_{13} - H_{11}H_{23} & | & H_{11}H_{22} - H_{12}^2 \end{pmatrix}.$$

Setting $\boldsymbol{B} = \boldsymbol{A}(\boldsymbol{A}^{\mathrm{T}}\boldsymbol{A})^{-1}$, the components of $\bar{\boldsymbol{\beta}} = \boldsymbol{B}^{\mathrm{T}}\bar{\boldsymbol{y}}$ are

$$\bar{\beta}_1 = \sum_{j=1}^{m} b_{j1}\bar{y}_j\,, \quad \bar{\beta}_2 = \sum_{j=1}^{m} b_{j2}\bar{y}_j\,, \quad \bar{\beta}_3 = \sum_{j=1}^{m} b_{j3}\bar{y}_j$$

or

$$\begin{aligned} \bar{\beta}_1 = \frac{1}{D}\sum_{j=1}^{m} \big\{ & \left[H_{22}H_{33} - H_{23}^2\right] + \left[H_{23}H_{13} - H_{12}H_{33}\right]\bar{x}_j \\ & + \left[H_{12}H_{23} - H_{22}H_{13}\right]\bar{x}_j^2 \big\}\,\bar{y}_j \end{aligned}$$

$$\bar{\beta}_2 = \frac{1}{D}\sum_{j=1}^{m}\left\{\left[H_{23}H_{13} - H_{12}H_{33}\right] + \left[H_{11}H_{33} - H_{13}^2\right]\bar{x}_j + \left[H_{12}H_{13} - H_{11}H_{23}\right]\bar{x}_j^2\right\}\bar{y}_j$$

$$\bar{\beta}_3 = \frac{1}{D}\sum_{j=1}^{m}\left\{\left[H_{12}H_{23} - H_{22}H_{13}\right] + \left[H_{12}H_{13} - H_{11}H_{23}\right]\bar{x}_j + \left[H_{11}H_{22} - H_{12}^2\right]\bar{x}_j^2\right\}\bar{y}_j\,.$$

The partial derivatives of the determinant follow from

$$\begin{aligned}\frac{\partial D}{\partial \bar{x}_i} &= 2\left[H_{13}H_{23} - H_{12}H_{33}\right] \\ &\quad +2\left[H_{11}H_{33} + 2\left(H_{12}H_{23} - H_{13}H_{22}\right) - H_{13}^2\right]\bar{x}_i \\ &\quad +6\left[H_{12}H_{13} - H_{11}H_{23}\right]\bar{x}_i^2 + 4\left(H_{11}H_{22} - H_{12}^2\right)\bar{x}_i^3 \\ \frac{\partial D}{\partial \bar{y}_i} &= 0\,,\end{aligned}$$

and for those of the components of the solution vector we have

$$\begin{aligned}c_{i1} = \frac{\partial \bar{\beta}_1}{\partial \bar{x}_i} &= -\frac{\bar{\beta}_1}{D}\frac{\partial D}{\partial \bar{x}_i} + \frac{1}{D}\left\{2\left(H_{33}\bar{x}_i - 3H_{23}\bar{x}_i^2 + 2H_{22}\bar{x}_i^3\right)\sum_{j=1}^{m}\bar{y}_j\right. \\ &\quad + \left(H_{23}H_{13} - H_{12}H_{33}\right)\bar{y}_i \\ &\quad + \left(-H_{33} + 2H_{23}\bar{x}_i + 3H_{13}\bar{x}_i^2 - 4H_{12}\bar{x}_i^3\right)\sum_{j=1}^{m}\bar{x}_j\bar{y}_j \\ &\quad +2\left(H_{12}H_{23} - H_{22}H_{13}\right)\bar{x}_i\bar{y}_i \\ &\quad \left. + \left[H_{23} - 2\left(H_{13} + H_{22}\right)\bar{x}_i + 3H_{12}\bar{x}_i^2\right]\sum_{j=1}^{m}\bar{x}_j^2\bar{y}_j\right\}\end{aligned}$$

$$c_{i+m,1} = \frac{\partial \bar{\beta}_1}{\partial \bar{y}_i} = b_{i1}$$

$$\begin{aligned}c_{i2} = \frac{\partial \bar{\beta}_2}{\partial \bar{x}_i} &= -\frac{\bar{\beta}_2}{D}\frac{\partial D}{\partial \bar{x}_i} + \frac{1}{D}\left\{\left(-H_{33} + 2H_{23}\bar{x}_i + 3H_{13}\bar{x}_i^2 - 4H_{12}\bar{x}_i^3\right)\sum_{j=1}^{m}\bar{y}_j\right. \\ &\quad +4\left(-H_{13}\bar{x}_i + H_{11}x_i^3\right)\sum_{j=1}^{m}\bar{x}_j\bar{y}_j \\ &\quad + \left(H_{11}H_{33} - H_{13}^2\right)\bar{y}_i + 2\left(H_{12}H_{13} - H_{11}H_{23}\right)\bar{x}_i\bar{y}_i \\ &\quad \left. + \left[H_{13} + 2H_{12}\bar{x}_i - 3H_{11}\bar{x}_i^2\right]\sum_{j=1}^{m}\bar{x}_j^2\bar{y}_j\right\}\end{aligned}$$

$$c_{i+m,2} = \frac{\partial \bar{\beta}_2}{\partial \bar{y}_i} = b_{i2}$$

$$c_{i3} = \frac{\partial \bar{\beta}_3}{\partial \bar{x}_i} = -\frac{\bar{\beta}_3}{D}\frac{\partial D}{\partial \bar{x}_i} + \frac{1}{D}\left\{ \left[H_{23} - 2\left(H_{13}+H_{22}\right)\bar{x}_i + 3H_{12}\bar{x}_i^2\right] \sum_{j=1}^{m} \bar{y}_j \right.$$

$$+ \left(H_{13} + 2H_{12}\bar{x}_i - 3H_{11}\bar{x}_i^2\right) \sum_{j=1}^{m} \bar{x}_j\bar{y}_j + \left(H_{12}H_{13} - H_{11}H_{23}\right)\bar{y}_i$$

$$\left. +2\left(H_{11}H_{22} - H_{12}^2\right)\bar{x}_i\bar{y}_i + 2\left(-H_{12} + H_{11}\bar{x}_i\right) \sum_{j=1}^{m} \bar{x}_j^2\bar{y}_j \right\}$$

$$c_{i+m,3} = \frac{\partial \bar{\beta}_3}{\partial \bar{y}_i} = b_{i3}\,.$$

Section 11.4: Circles

From

$$\boldsymbol{A} = \begin{pmatrix} 1 & \bar{u}_1 & \bar{v}_1 \\ 1 & \bar{u}_2 & \bar{v}_2 \\ \dots & \dots & \dots \\ 1 & \bar{u}_m & \bar{v}_m \end{pmatrix}$$

we find

$$\boldsymbol{A}^{\mathrm{T}}\boldsymbol{A} = \begin{pmatrix} H_{11} & H_{12} & H_{13} \\ H_{21} & H_{22} & H_{23} \\ H_{31} & H_{32} & H_{33} \end{pmatrix}$$

whose elements are given by

$$H_{11} = m\,, \qquad H_{22} = \sum_{j=1}^{m} \bar{u}_j^2\,, \qquad H_{33} = \sum_{j=1}^{m} \bar{v}_j^2$$

$$H_{12} = H_{21} = \sum_{j=1}^{m} \bar{u}_j\,, \quad H_{13} = H_{31} = \sum_{j=1}^{m} \bar{v}_j\,, \quad H_{23} = H_{32} = \sum_{j=1}^{m} \bar{u}_j\bar{v}_j\,.$$

The determinant of $\boldsymbol{A}^{\mathrm{T}}\boldsymbol{A}$ is

$$D = H_{11}\left(H_{22}H_{33} - H_{23}^2\right) + H_{12}\left(H_{31}H_{23} - H_{33}H_{12}\right) + H_{13}\left(H_{21}H_{32} - H_{13}H_{22}\right)\,.$$

so that

$$\left(\boldsymbol{A}^{\mathrm{T}}\boldsymbol{A}\right)^{-1} = \frac{1}{D}\begin{pmatrix} H_{22}H_{33} - H_{23}^2 & H_{23}H_{13} - H_{12}H_{33} & H_{12}H_{23} - H_{22}H_{13} \\ H_{23}H_{13} - H_{12}H_{33} & H_{11}H_{33} - H_{13}^2 & H_{12}H_{13} - H_{11}H_{23} \\ H_{12}H_{23} - H_{22}H_{13} & H_{12}H_{13} - H_{11}H_{23} & H_{11}H_{22} - H_{12}^2 \end{pmatrix}\,.$$

Putting $\boldsymbol{B} = \boldsymbol{A}(\boldsymbol{A}^{\mathrm{T}}\boldsymbol{A})^{-1}$ the components of $\bar{\boldsymbol{\beta}} = \boldsymbol{B}^{\mathrm{T}}\bar{\boldsymbol{w}}$ are

$$\bar{\beta}_1 = \sum_{j=1}^{m} b_{j1}\bar{w}_j\,, \quad \bar{\beta}_2 = \sum_{j=1}^{m} b_{j2}\bar{w}_j\,, \quad \bar{\beta}_3 = \sum_{j=1}^{m} b_{j3}\bar{w}_j$$

or

$$\begin{aligned}
\bar{\beta}_1 &= \frac{1}{D}\sum_{j=1}^{m}\left\{\left[H_{22}H_{33} - H_{23}^2\right] + \left[H_{23}H_{13} - H_{12}H_{33}\right]\bar{u}_j\right. \\
&\quad \left. + \left[H_{12}H_{23} - H_{22}H_{13}\right]\bar{v}_j\right\}\bar{w}_j \\
\bar{\beta}_2 &= \frac{1}{D}\sum_{j=1}^{m}\left\{\left[H_{23}H_{13} - H_{12}H_{33}\right] + \left[H_{11}H_{33} - H_{13}^2\right]\bar{u}_j\right. \\
&\quad \left. + \left[H_{12}H_{13} - H_{11}H_{23}\right]\bar{v}_j\right\}\bar{w}_j \\
\bar{\beta}_3 &= \frac{1}{D}\sum_{j=1}^{m}\left\{\left[H_{12}H_{23} - H_{22}H_{13}\right] + \left[H_{12}H_{13} - H_{11}H_{23}\right]\bar{u}_j\right. \\
&\quad \left. + \left[H_{11}H_{22} - H_{12}^2\right]\bar{v}_j\right\}\bar{w}_j\,.
\end{aligned}$$

For the partial derivatives of the determinant we find

$$\begin{aligned}
\frac{\partial D}{\partial \bar{x}_i} &= \frac{2}{r^*}\left[\left(H_{11}H_{33} - H_{13}^2\right)\bar{u}_i + \left(H_{13}H_{12} - H_{11}H_{23}\right)\bar{v}_i\right. \\
&\quad \left. + \left(H_{13}H_{23} - H_{33}H_{12}\right)\right] \\
\frac{\partial D}{\partial \bar{y}_i} &= \frac{2}{r^*}\left[\left(H_{12}H_{13} - H_{11}H_{23}\right)\bar{u}_i + \left(H_{11}H_{22} - H_{12}^2\right)\bar{v}_i\right. \\
&\quad \left. + \left(H_{12}H_{23} - H_{13}H_{22}\right)\right]
\end{aligned}$$

and for those of the components of the solution vector

$$\begin{aligned}
c_{i1} = \frac{\partial \bar{\beta}_1}{\partial \bar{x}_i} &= -\frac{\bar{\beta}_1}{D}\frac{\partial D}{\partial \bar{x}_i} + \frac{1}{D}\left\{\frac{2}{r^*}\left(H_{33}\bar{u}_i - H_{23}\bar{v}_i\right)\sum_{j=1}^{m}\bar{w}_j\right. \\
&\quad + \left(H_{22}H_{33} - H_{23}^2\right)\bar{u}_i \\
&\quad + \frac{1}{r^*}\left(H_{13}\bar{v}_i - H_{33}\right)\sum_{j=1}^{m}\bar{u}_j\bar{w}_j + \left(H_{23}H_{13} - H_{12}H_{33}\right)\left(\frac{\bar{w}_i}{r^*} + \bar{u}_i^2\right) \\
&\quad \left. + \frac{1}{r^*}\left(H_{23} + H_{12}\bar{v}_i - 2H_{13}\bar{u}_i\right)\sum_{j=1}^{m}\bar{v}_j\bar{w}_j + \left(H_{12}H_{23} - H_{22}H_{13}\right)\bar{u}_i\bar{v}_i\right\} \\
c_{i+m,1} = \frac{\partial \bar{\beta}_1}{\partial \bar{y}_i} &= -\frac{\bar{\beta}_1}{D}\frac{\partial D}{\partial \bar{y}_i} + \frac{1}{D}\left\{\frac{2}{r^*}\left(H_{22}\bar{v}_i - H_{23}\bar{u}_i\right)\sum_{j=1}^{m}\bar{w}_j\right. \\
&\quad + \left(H_{22}H_{33} - H_{23}^2\right)\bar{v}_i
\end{aligned}$$

$$
\begin{aligned}
&+\frac{1}{r^*}\left(H_{13}\bar{u}_i + H_{23} - 2H_{12}\bar{v}_i\right)\sum_{j=1}^{m}\bar{u}_j\bar{w}_j + \left(H_{23}H_{13} - H_{12}H_{33}\right)\bar{u}_i\bar{v}_i \\
&+\frac{1}{r^*}\left(H_{12}\bar{u}_i - H_{22}\right)\sum_{j=1}^{m}\bar{v}_j\bar{w}_j + \left(H_{12}H_{23} - H_{22}H_{13}\right)\left(\frac{\bar{w}_i}{r^*} + \bar{v}_i^2\right)\Bigg\} \\
c_{i2} = \frac{\partial\bar{\beta}_2}{\partial\bar{x}_i} &= -\frac{\bar{\beta}_2}{D}\frac{\partial D}{\partial\bar{x}_i} + \frac{1}{D}\Bigg\{\frac{1}{r^*}\left(H_{13}\bar{v}_i - H_{33}\right)\sum_{j=1}^{m}\bar{w}_j \\
&+\left(H_{23}H_{13} - H_{12}H_{33}\right)\bar{u}_i + \left(H_{11}H_{33} - H_{13}^2\right)\left(\frac{\bar{w}_i}{r^*} + \bar{u}_i^2\right) \\
&+\frac{1}{r^*}\left(H_{13} + H_{11}\bar{v}_i\right)\sum_{j=1}^{m}\bar{v}_j\bar{w}_j + \left(H_{12}H_{13} - H_{11}H_{23}\right)\bar{u}_i\bar{v}_i\Bigg\} \\
c_{i+m,2} = \frac{\partial\bar{\beta}_2}{\partial\bar{y}_i} &= -\frac{\bar{\beta}_2}{D}\frac{\partial D}{\partial\bar{y}_i} + \frac{1}{D}\Bigg\{\frac{1}{r^*}\left(H_{23} + H_{13}\bar{u}_i - 2H_{12}\bar{v}_i\right)\sum_{j=1}^{m}\bar{w}_j \\
&+\left(H_{23}H_{13} - H_{12}H_{33}\right)\bar{v}_i \\
&+\frac{2}{r^*}\left(H_{11}\bar{v}_i - H_{13}\right)\sum_{j=1}^{m}\bar{u}_j\bar{w}_j + \left(H_{11}H_{33} - H_{13}^2\right)\bar{u}_i\bar{v}_i \\
&+\frac{1}{r^*}\left(H_{12} - H_{11}\bar{u}_i\right)\sum_{j=1}^{m}\bar{v}_j\bar{w}_j + \left(H_{12}H_{13} - H_{11}H_{23}\right)\left(\frac{\bar{w}_i}{r^*} + \bar{v}_i^2\right)\Bigg\} \\
c_{i3} = \frac{\partial\bar{\beta}_3}{\partial\bar{x}_i} &= -\frac{\bar{\beta}_3}{D}\frac{\partial D}{\partial\bar{x}_i} + \frac{1}{D}\Bigg\{\frac{1}{r^*}\left(H_{23} + H_{12}\bar{v}_i - 2H_{13}\bar{u}_i\right)\sum_{j=1}^{m}\bar{w}_j \\
&+\left(H_{12}H_{23} - H_{22}H_{13}\right)\bar{u}_i + \frac{1}{r^*}\left(H_{13} - H_{11}\bar{v}_i\right)\sum_{j=1}^{m}\bar{u}_j\bar{w}_j \\
&+\left(H_{12}H_{13} - H_{11}H_{23}\right)\left(\frac{\bar{w}_i}{r^*} + \bar{u}_i^2\right) + \frac{2}{r^*}\left(H_{11}\bar{u}_i - H_{12}\right)\sum_{j=1}^{m}\bar{v}_j\bar{w}_j \\
&+\left(H_{11}H_{22} - H_{12}^2\right)\bar{u}_i\bar{v}_i\Bigg\} \\
c_{i+m,3} = \frac{\partial\bar{\beta}_3}{\partial\bar{y}_i} &= -\frac{\bar{\beta}_3}{D}\frac{\partial D}{\partial\bar{y}_i} + \frac{1}{D}\Bigg\{\frac{1}{r^*}\left(H_{12}\bar{u}_i - H_{22}\right)\sum_{j=1}^{m}\bar{w}_j \\
&+\left(H_{12}H_{23} - H_{22}H_{13}\right)\bar{v}_i + \frac{1}{r^*}\left(H_{12} - H_{11}\bar{u}_i\right)\sum_{j=1}^{m}\bar{u}_j\bar{w}_j \\
&+\left(H_{12}H_{13} - H_{11}H_{23}\right)\bar{u}_i\bar{v}_i + \left(H_{11}H_{22} - H_{12}^2\right)\left(\frac{\bar{w}_i}{r^*} + \bar{v}_i^2\right)\Bigg\}\,.
\end{aligned}
$$

G Student's Density

Suppose the random variable X to be $N(\mu, \sigma^2)$-distributed. Then, its distribution function is given by

$$P(X \leq x) = \frac{1}{\sigma\sqrt{2\pi}} \int_{-\infty}^{x} \exp\left(-\frac{(x-\mu)^2}{2\sigma^2}\right) \mathrm{d}x\,. \tag{G.1}$$

We consider a sample

$$x_1, x_2, \ldots, x_n \tag{G.2}$$

and the estimator

$$s^2 = \frac{1}{n-1} \sum_{l=1}^{n} (x_l - \bar{x})^2\ ; \quad \nu = n-1\,. \tag{G.3}$$

For a fixed t we define

$$x = \mu + ts\,, \tag{G.4}$$

so that

$$P(X \leq \mu + ts) = \frac{1}{\sigma\sqrt{2\pi}} \int_{-\infty}^{\mu+ts} \exp\left(-\frac{(x-\mu)^2}{2\sigma^2}\right) \mathrm{d}x\,. \tag{G.5}$$

Substituting $\eta = (x-\mu)/\sigma$ for x leads to

$$P(X \leq \mu + ts) = P(t, s, \nu) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{ts/\sigma} \mathrm{e}^{-\eta^2/2} \mathrm{d}\eta\,. \tag{G.6}$$

For this statement to be statistically representative, we average by means of the density

$$p_{S^2}\left(s^2\right) = \frac{\nu^{\nu/2}}{2^{\nu/2}\Gamma(\nu/2)\,\sigma^{\nu}} \exp\left(-\frac{\nu s^2}{2\sigma^2}\right) s^{\nu-2}\,, \tag{G.7}$$

which we deduce from (3.36) putting $\chi^2 = \frac{n-1}{\sigma^2}s^2$ and $p_{S^2}(s^2) = p_{\chi^2}\frac{d\chi^2}{ds^2}$, so that

$$P(t,\nu) = E\{P(t,s,\nu)\} = \int_0^\infty \left\{ \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{ts/\sigma} \mathrm{e}^{-\eta^2/2} \mathrm{d}\eta \right\} p_{S^2}\left(s^2\right) \mathrm{d}s^2 \,. \quad \text{(G.8)}$$

Averaging by means of the density $p_S(s)$ as given e.g. in [50] leads to the same result as $p_S(s)ds = p_{S^2}(S^2)dS^2$.

Obviously, (G.8) is a distribution function and its only variable is t. Hence, differentiating with respect to t,

$$\frac{\mathrm{d}P(t,\nu)}{\mathrm{d}t} = \int_0^\infty \left\{ \frac{1}{\sigma\sqrt{2\pi}} \exp\left(-\frac{t^2 s^2}{2\sigma^2}\right) s \right\} p_{S^2}\left(s^2\right) \mathrm{d}s^2 \,, \quad \text{(G.9)}$$

and integrating out the right hand side, we find Student's (or Gosset's) density

$$p_T(t,\nu) = \frac{\Gamma\left(\frac{\nu+1}{2}\right)}{\sqrt{\pi\nu}\Gamma\left(\frac{\nu}{2}\right)} \frac{1}{\left(1+\frac{t^2}{\nu}\right)^{\frac{\nu+1}{2}}} \quad \text{(G.10)}$$

the random variable of which is implied in (G.4),

$$T(\nu) = \frac{X-\mu}{S} \,. \quad \text{(G.11)}$$

According to (G.7), the number of the degrees of freedom is $\nu = n-1$. Instead of (G.2) we now consider the estimator

$$\bar{x} = \frac{1}{n}\sum_{l=1}^{n} \bar{x}_l \quad \text{(G.12)}$$

and the limit of integration

$$\bar{x} = \mu + ts/\sqrt{n} \quad \text{(G.13)}$$

so that

$$P\left(\bar{X} \le \bar{x}\right) = \frac{1}{\sigma/\sqrt{n}\sqrt{2\pi}} \int_{-\infty}^{\bar{x}} \exp\left(-\frac{(\bar{x}-\mu)^2}{2\sigma^2/n}\right) \mathrm{d}\bar{x} \quad \text{(G.14)}$$

leads us to

$$P\left(\bar{X} \le \mu + ts/\sqrt{n}\right) = \frac{1}{\sigma/\sqrt{n}\sqrt{2\pi}} \int_{-\infty}^{\mu+ts/\sqrt{n}} \exp\left(-\frac{(\bar{x}-\mu)^2}{2\sigma^2/n}\right) \mathrm{d}\bar{x} \,. \quad \text{(G.15)}$$

On substituting $\eta = (\bar{x} - \mu)/(\sigma/\sqrt{n})$ we again arrive at (G.6). Hence, the random variable

$$T(\nu) = \frac{\bar{X} - \mu}{S/\sqrt{n}}\,. \tag{G.16}$$

is t-distributed with $\nu = n - 1$ degrees of freedom.

H Quantiles of Hotelling's Density

$t_{0.95}$; P=95%

m/n	1	2	3	4	5	6	7	8	9	10
1										
2	13									
3	4.3	28								
4	3.2	7.6	44							
5	2.8	5.1	10.7	60						
6	2.6	4.2	6.8	13.9	76					
7	2.5	3.7	5.4	8.5	17.0	92				
8	2.4	3.5	4.8	6.7	10.3	20.1	108			
9	2.3	3.3	4.4	5.8	7.9	12.0	23.3	124		
10	2.3	3.2	4.1	5.2	6.7	9.1	13.7	26.4	140	
11	2.2	3.1	3.9	4.9	6.0	7.7	10.3	15.4	29.5	156
12	2.2	3.0	3.8	4.6	5.6	6.9	8.7	11.5	17.1	32.7
13	2.2	3.0	3.7	4.4	5.3	6.3	7.7	9.6	12.7	18.8
14	2.2	2.9	3.6	4.3	5.0	5.9	7.0	8.5	10.6	13.9
15	2.1	2.9	3.5	4.1	4.8	5.6	6.6	7.7	9.3	11.2
16	2.1	2.8	3.4	4.0	4.7	5.4	6.2	7.2	8.4	10.1
17	2.1	2.8	3.4	4.0	4.6	5.2	5.9	6.8	7.8	9.1
18	2.1	2.8	3.3	3.9	4.5	5.1	5.7	6.5	7.4	8.4
19	2.1	2.8	3.3	3.8	4.4	4.9	5.5	6.2	7.0	7.9
20	2.1	2.7	3.3	3.8	4.3	4.8	5.4	6.0	6.7	7.5
21	2.1	2.7	3.3	3.7	4.2	4.7	5.3	5.8	6.5	7.2
22	2.1	2.7	3.2	3.7	4.2	4.7	5.2	5.7	6.3	6.9
23	2.1	2.7	3.2	3.7	4.1	4.6	5.1	5.6	6.1	6.7
24	2.1	2.7	3.2	3.6	4.1	4.5	5.0	5.5	6.0	6.5
25	2.1	2.7	3.2	3.6	4.0	4.5	4.9	5.4	5.9	6.4
26	2.1	2.7	3.1	3.6	4.0	4.4	4.8	5.3	5.7	6.2
27	2.1	2.7	3.1	3.6	4.0	4.4	4.8	5.2	5.7	6.1
28	2.1	2.7	3.1	3.5	3.9	4.3	4.7	5.1	5.6	6.0
29	2.1	2.6	3.1	3.5	3.9	4.3	4.7	5.1	5.5	5.9
30	2.0	2.6	3.1	3.5	3.9	4.3	4.6	5.0	5.4	5.8
31	2.0	2.6	3.1	3.5	3.9	4.2	4.6	5.0	5.4	5.8
32		2.6	3.1	3.5	3.8	4.2	4.6	4.9	5.3	5.7
33			3.1	3.5	3.8	4.2	4.5	4.9	5.3	5.6
34				3.4	3.8	4.2	4.5	4.9	5.2	5.6
35					3.8	4.1	4.5	4.8	5.2	5.5
36						4.1	4.5	4.8	5.1	5.4
37							4.4	4.7	5.1	5.4
38								4.7	5.1	5.4
39									5.0	5.3
40										5.3

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