Accounting for correlations in measurement models

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Examples of Measurement Uncertainty Evaluation

Introduction

- Correlations (dependencies) between quantities arise when they depend on (at least) one other joint quantity
- It is essential to evaluate covariances as part of the evaluation of measurement uncertainty
- Ignoring covariances is the same as setting them to zero ...
- ... which may lead to serious over- or understating the measurement uncertainty

Contents

A simple case

- A calibrated volt meter is used to measure two voltages which are to be used in a subsequent calculation. What is the covariance between the two voltages?
  - $V_1 = \delta V_{\text{cal}} + \bar{V}_{\text{ind},1}$
  - $V_2 = \delta V_{\text{cal}} + \bar{V}_{\text{ind},2}$
- We assume the indications as independent and identically distributed (IID).
- The only common variable in the two measurement equations is δV_{cal}, so according to equation (F.2) in the GUM, $u(V_1, V_2) = u^2(\delta V_{\text{cal}})$
- The correlation coefficient is evaluated as $r(V_1, V_2) = \dfrac{u^2(\delta V_{\text{cal}})}{u(V_1)u(V_2)}$

Generalisation to multiple common quantities

- If there are multiple common input quantities,

$$u(X_1, X_2) = \sum_i \frac{\partial F}{\partial Q_i} \frac{\partial G}{\partial Q_i} u^2(Q_i)$$

- where F and G are the measurement equations relating X_1 and X_2 to the input quantities Q_i;
- only terms for which both partial derivatives are non-zero contribute (i.e., the ones concerning the common quantities).
- See also JCGM 100:2008 clause F.1.2

Buoyancy effect on a permeation tube in a chamber flushed with high-purity nitrogen

- Measurand of interest: permeation rate $\dot{m} = q_m = \mathrm{d}m/\mathrm{d}t$
- Buoyancy effect used to model temperature and pressure influence on weighing results
- Buoyancy effect modelled as

$$\delta m_{\mathrm{buo}} = V_{\mathrm{tube}} \delta\rho \qquad \text{where} \qquad \rho = \frac{\bar{M}}{V_{\mathrm{m}}}$$

- Molar volume of high-purity nitrogen V_{m} computed using a cubic polynomial (Soave-Redlich-Kwong equation-of-state)

Use of the Soave-Redlich-Kwong equation-of-state

Equation-of-state can be formulated as

$$V_m^3 + \alpha_1 V_m^2 + \alpha_2 V_m + \alpha_3 = 0$$

where

$$\alpha_1 = -\frac{RT}{p}; \alpha_2 = -b^2 - \frac{RT}{p} b + \frac{a}{p}; \alpha_3 = -\frac{ab}{p}$$

and a and b are coefficients dependent on, among other, the critical temperature and pressure.

Propagation of uncertainty can be performed using the law of propagation of uncertainty from GUM-S2 for (multivariate) implicit measurement models, enabling including the correlations between the α_i, i.e.,

$$u^2(V_\mathrm{m}) = \left(3V_\mathrm{m}^2 + 2\alpha_1 V_\mathrm{m} + \alpha_2\right)^{-2} \boldsymbol{C}_{\boldsymbol{\alpha}} \boldsymbol{U}_{\boldsymbol{\alpha}} \boldsymbol{C}_{\boldsymbol{\alpha}}^\mathrm{T}$$

Generalisation to multiple output quantities

- If there are
  - multiple quantities having correlations and/or
  - multiple measurement equations

  the law of propagation of uncertainty for multivariate measurement models (GUM-S2) is a convenient tool to calculate the covariances
- In the notation from the GUM, let $X_i = f_i(\boldsymbol{Q})$ for $i = 1 \dots N$, then $\boldsymbol{U_X} = \boldsymbol{C}\boldsymbol{U_Q}\boldsymbol{C}^\top$ provides a full covariance matrix $\boldsymbol{U_X}$, containing all covariances $u(X_i, X_j)$.
- The matrix $\boldsymbol{C}$ holds the sensitivity coefficients $\partial f_i / \partial Q_j$

Normalisation of a composition

- The composition of any material, expressed in fractions always adds up to a constant
- Hence, these fractions are always correlated and the uncertainty of the sum of all fractions is always zero
- Suppose we have N raw amount fractions $x_1, \ldots, x_N$
- Then the composition expressed in amount fractions is given by $y_i = x_i / \sum_j x_j$
- From this expression, it is clear that any y_i depends on all x_j
- Other cases lead to other uncertainty structures, but still there are covariances to be taken into account

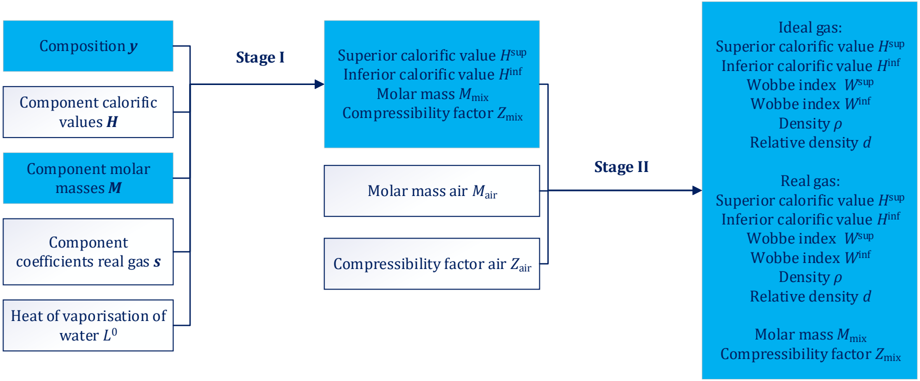
Effect of ignoring covariances in calculation of natural gas properties

Table: Natural gas properties calculated from ISO 6976:2016, example 3

	Ignoring correlations			Including correlations		
	x	$u(x)$	$u_{\mathrm{rel}}(x)$	x	$u(x)$	$u_{\mathrm{rel}}(x)$
H	937.14	0.63	0.067 %	937.14	0.38	0.040 %
$\bar{M}$	18.035	0.014	0.076 %	18.035	0.006	0.035 %
Z	0.997 57	0.000 05	0.005 %	0.997 57	0.000 05	0.005 %

Standard uncertainties calculated for the superior calorific value (H) and molar mass ($\bar{M}$) vastly different; effect of ignoring correlations differs on a case-by-case basis

Multistage measurement models with correlated input quantities: natural gas properties (ISO 6976)



Multistage measurement models with correlated input quantities: natural gas properties (ISO 6976)

- Use of law of propagation of uncertainty from GUM-S2 provides a computationally efficient way to propagate measurement uncertainty
- Appendix B of ISO 6976:2016 provides, without matrix calculus, all expressions to calculate the uncertainties associated with the natural gas properties
- It does not provide expressions for the covariances between natural gas properties, . . .
- . . . but these are often required in subsequent applications (such as calculating measurement errors).
- Duly propagating uncertainty in this area requires substantial mathematical skills, often not available to the readership of the standard.

Autocorrelation

- JCGM 100 presumes that correlations can be dealt with by expressing input quantities into a further set of (uncorrelated) input quantities
- Temperature readings of the thermocouple are *serially* correlated due to the working of the heater of the thermal bath
- A time series analysis is an appropriate way to deal with this form of correlation

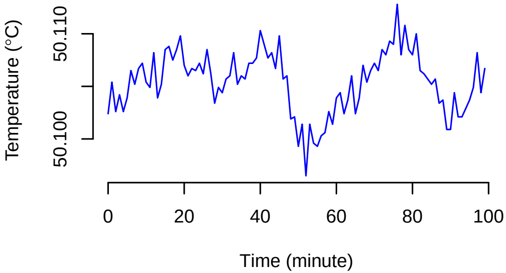


Figure: Readings of a thermocouple measuring the temperature of a thermal bath (JCGM 103:202n)

Autocorrelation (continued)

- In this instance, an auto-regression of order 2 is an appropriate model for the data
- A naive type A evaluation of standard uncertainty would yield $u(t) = 0.0003\,°\mathrm{C}$, whereas an ARIMA(2,0,0) model provides $u(t) = 0.0010\,°\mathrm{C}$, thus about three times larger (see JCGM 103:202n)

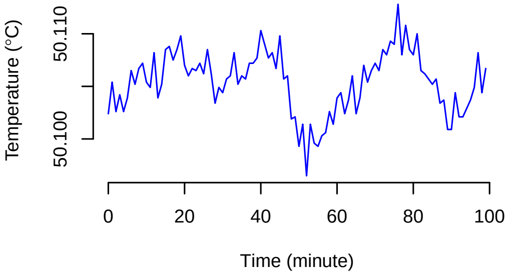


Figure: Readings of a thermocouple measuring the temperature of a thermal bath (JCGM 103:202n)

Regression

- Coefficients of a regression model are almost always correlated
- Consider the generalised linear model $y = \sum_i a_i \phi_i(x)$ where $\phi_i(x)$ is some function of i,
- the measurement model is (often) implicit, relating the a_i to a set of pairwise (x_j, y_j) values and corresponding uncertainties; there can be correlations between pairs of (x_j, x_k), (y_j, y_k) and (x_j, y_j) too.
- Any good software package provides a full covariance matrix
- Use of multiple coefficients in a subsequent calculation requires information of the corresponding covariances
- See also example 9.5 in GUM-S2 (temperature from a resistance thermometer)

Monte Carlo method and Bayesian inference

- Correlations between input quantities modelled by either
  - expressing these in independent quantities and assigning probability density functions
  - assigning a joint probability density function (such as the multivariate normal, t, or Dirichlet distribution)
- Not for all univariate probability density functions there is a multivariate counterpart (e.g., rectangular distribution)
- GUM-S2, section 7.6 provides an expression for obtaining the covariance matrix $\boldsymbol{U}_{\boldsymbol{y}}$ associated with the output vector $\boldsymbol{y}$
- Correlation matrix can be obtained as $\boldsymbol{R}_{\boldsymbol{y}} = \boldsymbol{D}\boldsymbol{U}_{\boldsymbol{y}}\boldsymbol{D}$ where $\boldsymbol{D} = \mathrm{diag}\{u^{-1}(y_1), \ldots, u^{-1}(y_M)\}$
- Approaches for Bayesian inference are very similar (including for assigning (joint) prior probability density functions)

Bayesian EIV regression

- From a Markov Chain Monte Carlo calculation, the coefficients of a straight line (errors-in-variables regression) are obtained
- If the coefficients are to be communicated, the associated covariance matrix should be provided as well
- This covariance matrix can obtained from the MCMC samples of the calculation as described in GUM-S2
- MCMC examples can be extracted from the calculation

Table: Results from fitting the Bayesian model for EIV for standard addition

	mean	sd	2.5 %	97.5 %
a	10.28	8.22	1.16	30.52
b	26.75	1.30	23.69	29.07
$r_{x,1}$	0.01	1.00	−1.95	1.97
$r_{x,2}$	−0.02	1.00	−1.98	1.94
$r_{x,3}$	0.01	1.00	−1.95	1.97
$r_{y,1}$	0.02	0.75	−0.79	1.83
$r_{y,2}$	0.37	0.87	−0.58	2.35
$r_{y,3}$	0.03	1.18	−2.04	2.49
y_1	0.39	0.35	0.04	1.24

Concluding remarks

- Evaluating covariances is an essential part of any uncertainty evaluation; they can increase or decrease the computed uncertainty
- When properly established, a measurement model articulates the dependencies between variables
- It is not always necessary to express the measurand(s) into a set of uncorrelated input quantities
- Working with multivariate methods (GUM-S2) is often the easier choice, but requires familiarity with matrix calculus
- Monte Carlo method and MCMC also provide means to extract information about covariances between output quantities

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EMUE Examples of Measurement Uncertainty Evaluation

EMPIR EURAMET

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