

Bayesian Statistics and AI

How they transform analytical measurements: why measurement uncertainty is more than a single number, and why correlated errors matter

Erik van der Werff · Qualimetric · Version 1.0 · October 2026 · First published on qualimetric.eu, 23 May 2025

Summary

Even the most precise analytical instruments are subject to measurement uncertainty, and traditional statistical methods struggle when the uncertainties of input variables are correlated. Bayesian statistics replace single-value estimates by full probability distributions, make prior knowledge and covariances explicit, and, combined with AI and modern computing, turn complex measurement data into reliable decisions. This paper explains why covariances between input quantities matter, how Bayesian models account for them, and what that means for laboratories that have to defend their results.

1. From point estimates to probability distributions

In the world of analytical measurements, accuracy has always been the holy grail. Yet even the most precise instruments are subject to measurement uncertainty, a reality that, until recently, has been difficult to handle rigorously. Traditional statistical methods often struggle when dealing with complex data structures or when the uncertainties in input variables are significantly correlated. But thanks to advances in Bayesian statistics, artificial intelligence (AI) and high-performance computing, we are now entering the era of reliability in data analysis.

Bayesian methods provide a powerful framework for incorporating prior knowledge and explicitly modelling uncertainty. Unlike classical approaches that produce single-value estimates, Bayesian analysis yields full posterior probability distributions, offering deeper insight into the reliability and variability of measurement results. This probabilistic perspective enables analysts to make better-informed decisions, especially in high-stakes applications where understanding the range of possible outcomes is as important as identifying the most likely one.

This is particularly valuable when dealing with covariances in input variables, where errors in measurements are not independent but structurally related. Classical regression techniques typically assume that the uncertainty of each variable is isolated. In contrast, Bayesian models allow us to include these interdependencies explicitly in the model structure, leading to more accurate inferences and better-calibrated predictions. As a result, measurement data that might previously have been discarded or oversimplified because of its complexity can now be fully used.

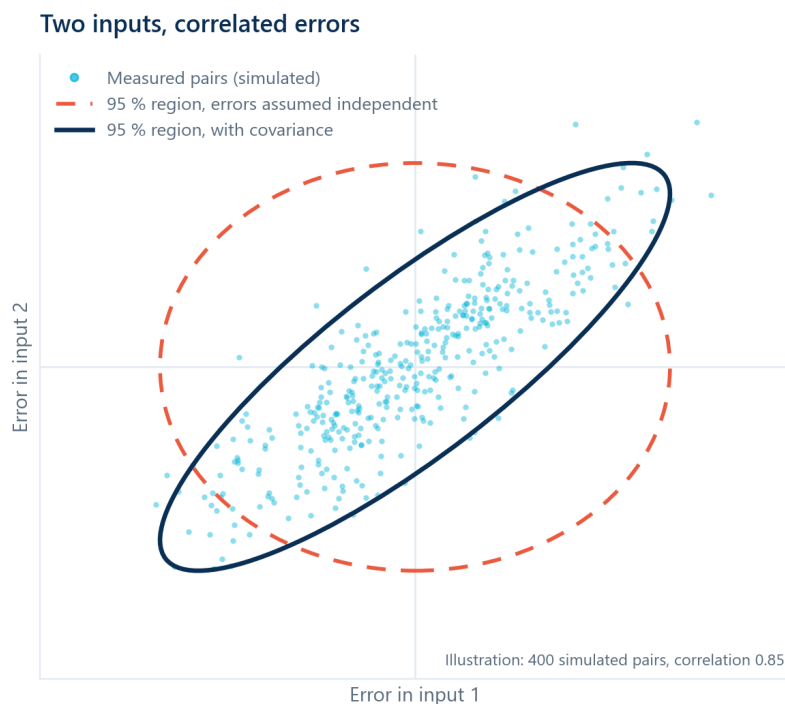


Figure 1. Two inputs with correlated errors. The 95 % region with covariance is a narrow, tilted ellipse; assuming independent errors gives a wide ellipse that is too large in one direction and too small in the other.

Covariance is a measure of how two variables vary together, and it becomes especially important when both variables are used as inputs in a model. In such cases their measurement uncertainties may be statistically related: an overestimation in one may often coincide with an overestimation in the other. Accounting for this mutual uncertainty is crucial for realistic and reliable model outcomes. This differs from the typical use of covariance in regression, where one variable is treated as an input and the other as an output. When both are inputs, it is not about cause and effect, but about capturing the interdependence of errors.

2. Why covariances matter

In real-world systems, especially in chemical, physical and environmental monitoring, input variables often show strong correlations. Ignoring these correlations can lead to underestimated uncertainties or even misleading conclusions. Bayesian models allow us to integrate the full covariance matrices of the measured variables directly into the inferential process, leading to more robust and realistic quantification of uncertainty.

3. The role of AI in uncertainty modelling

AI and machine learning models are increasingly used to model complex nonlinear systems. However, they have traditionally lacked a rigorous way to handle input uncertainty. Recent developments now allow Bayesian frameworks to be combined with neural networks and other AI tools, enabling models that learn from data while quantifying the uncertainty of their predictions: critical for decision-making in regulated industries such as energy, pharma, healthcare and analytical chemistry.

4. From data to decisions

As analytical instruments become more precise and data-rich, the challenge is no longer just in collecting data but in interpreting it reliably. The convergence of Bayesian statistics, AI and GPU computing offers a powerful pathway to extract more value from complex data, especially when measurement uncertainty and data correlation cannot be ignored.

It is time we embrace these tools not as academic luxuries, but as essential components of modern measurement science.

5. How NexChrom and GasCatena apply this

NexChrom, Qualimetric's software for handling gas chromatography data, calibrates with errors-in-variables regression following ISO 6143, which weighs the uncertainty of both the certified concentrations and the measured responses, and carries the full covariance of the calibration coefficients into every mole fraction. GasCatena, Qualimetric's software for the gravimetric preparation of calibration gases, propagates the covariance that normalisation creates between the mole fractions of a prepared gas into its ISO 6976 properties, so that a calorific value is neither inflated nor understated. More information and demonstrations are available at nexchrom.nl.

About the author

Erik van der Werff has worked for 25 years as an independent consultant in gas analysis, chemometrics and measurement uncertainty through Qualimetric. He is a member of ISO/TC 193/SC 1 (natural gas analysis), ISO/TC 28/WG 2 (precision of test methods) and ASTM D02, and the author of ISO 4259-5. He develops NexChrom. · qualimetric.eu · nexchrom.nl