International Standard

ISO 11843-6

Third edition
2025-10

Capability of detection —

Part 6: Methodology for the determination of the critical value and the minimum detectable value in Poisson distributed measurements by normal approximations

Capacité de détection —

Partie 6: Méthodologie pour la détermination de la valeur critique et de la valeur minimale détectable pour les mesures distribuées selon la loi de Poisson approximée par la loi Normale

Reference number
ISO 11843-6:2025(en)

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Published in Switzerland

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Foreword

ISO (the International Organization for Standardization) is a worldwide federation of national standards bodies (ISO member bodies). The work of preparing International Standards is normally carried out through ISO technical committees. Each member body interested in a subject for which a technical committee has been established has the right to be represented on that committee. International organizations, governmental and non-governmental, in liaison with ISO, also take part in the work. ISO collaborates closely with the International Electrotechnical Commission (IEC) on all matters of electrotechnical standardization.

The procedures used to develop this document and those intended for its further maintenance are described in the ISO/IEC Directives, Part 1. In particular, the different approval criteria needed for the different types of ISO document should be noted. This document was drafted in accordance with the editorial rules of the ISO/IEC Directives, Part 2 (see www.iso.org/directives).

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For an explanation of the voluntary nature of standards, the meaning of ISO specific terms and expressions related to conformity assessment, as well as information about ISO's adherence to the World Trade Organization (WTO) principles in the Technical Barriers to Trade (TBT), see www.iso.org/iso/foreword.html.

This document was prepared by Technical Committee ISO/TC 69, *Application of statistical methods*, Subcommittee SC 6, *Measurement methods and results*.

This third edition cancels and replaces the second edition (ISO 11843-6:2019), which has been technically revised.

The main changes are as follows:

— the symbols were modified to conform to ISO 11843-1;

— a list of symbols was moved from Annex A to Clause 4;

— in 6.3, explanatory text of how to determine the minimum detectable value was added;

— Clause 8 was revised to provide a description of the appropriate approach for determining whether or not the target substance has been detected;

— typographic and obvious errors were corrected.

A list of all parts in the ISO 11843 series can be found on the ISO website.

Any feedback or questions on this document should be directed to the user’s national standards body. A complete listing of these bodies can be found at www.iso.org/members.html.

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Introduction

Many types of instruments use the pulse-counting method for detecting signals. X-ray, electron and ion-spectroscopy detectors, such as X-ray diffractometers (XRD), X-ray fluorescence spectrometers (XRF), X-ray photoelectron spectrometers (XPS), Auger electron spectrometers (AES), secondary ion mass spectrometers (SIMS) and gas chromatograph mass spectrometers (GCMS) are of this type. These signals consist of a series of pulses produced at random and irregular intervals. They can be understood statistically using a Poisson distribution and the methodology for determining the minimum detectable value can be deduced from statistical principles.

Determining the minimum detectable value of signals is sometimes important in practical work. The value provides a criterion for deciding when "the signal is certainly not detected", or when "the signal is significantly different from the background noise level"[1]to[8]. For example, it is valuable when measuring the presence of hazardous substances or surface contamination of semi-conductor materials. RoHS (Restrictions on Hazardous Substances) sets limits on the use of six hazardous materials (hexavalent chromium, lead, mercury, cadmium and the flame retardant agents, perbromobiphenyl, PBB, and perbromodiphenyl ether, PBDE) in the manufacturing of electronic components and related goods sold in the EU. For that application, XRF and GCMS are the testing instruments used. XRD is used to measure the level of hazardous asbestos and crystalline silica present in the environment or in building materials.

Although the methodology employed to determine the minimum detection values has long been established in the field of chemical analysis, it has hitherto remained undefined within the domain of pulse count measurements. The necessity of establishing a methodology for determining the minimum detectable value in this field is duly acknowledged[9].

In this document the Poisson distribution is approximated by the normal distribution, ensuring consistency with the IUPAC approach laid out in the ISO 11843 series. The conventional approximation is used to generate the variance, the critical value of the response variable, the capability of detection criteria and the minimum detectability level[10].

In this document:

— α is the probability of erroneously detecting that a system is not in the basic state, when really it is in that state;

— β is the probability of erroneously not detecting that a system is not in the basic state when the value of the state variable is equal to the minimum detectable value(x_D).

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Capability of detection —

Part 6:
Methodology for the determination of the critical value and the minimum detectable value in Poisson distributed measurements by normal approximations

1 Scope

This document presents methods for determining the critical value of the response variable and the minimum detectable value in Poisson distribution measurements. It is applicable when variations in both the background noise and the signal are describable by the Poisson distribution. The conventional approximation is used to approximate the Poisson distribution by the normal distribution consistent with ISO 11843-3 and ISO 11843-4.

The accuracy of the normal approximation as compared to the exact Poisson distribution is discussed in Annex B.

2 Normative references

The following documents are referred to in the text in such a way that some or all of their content constitutes requirements of this document. For dated references, only the edition cited applies. For undated references, the latest edition of the referenced document (including any amendments) applies.

ISO Guide 30, *Reference materials — Selected terms and definitions*

ISO 3534-1, *Statistics — Vocabulary and symbols — Part 1: General statistical terms and terms used in probability*

ISO 11843-1, *Capability of detection — Part 1: Terms and definitions*

ISO 11843-2, *Capability of detection — Part 2: Methodology in the linear calibration case*

ISO 11843-3, *Capability of detection — Part 3: Methodology for determination of the critical value for the response variable when no calibration data are used*

ISO 11843-4, *Capability of detection — Part 4: Methodology for comparing the minimum detectable value with a given value*

3 Terms and definitions

For the purposes of this document, the terms and definitions given in ISO 3534-1, ISO 11843-1, ISO 11843-2, ISO 11843-3, ISO 11843-4, and ISO Guide 30 apply.

ISO and IEC maintain terminology databases for use in standardization at the following addresses:

— ISO Online browsing platform: available at https://www.iso.org/obp

— IEC Electropedia: available at https://www.electropedia.org/

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