MECA0010 – Reliability and stochastic modeling of engineered systems

Uncertainty quantification

Part 1 of 4 — Functions of random variables

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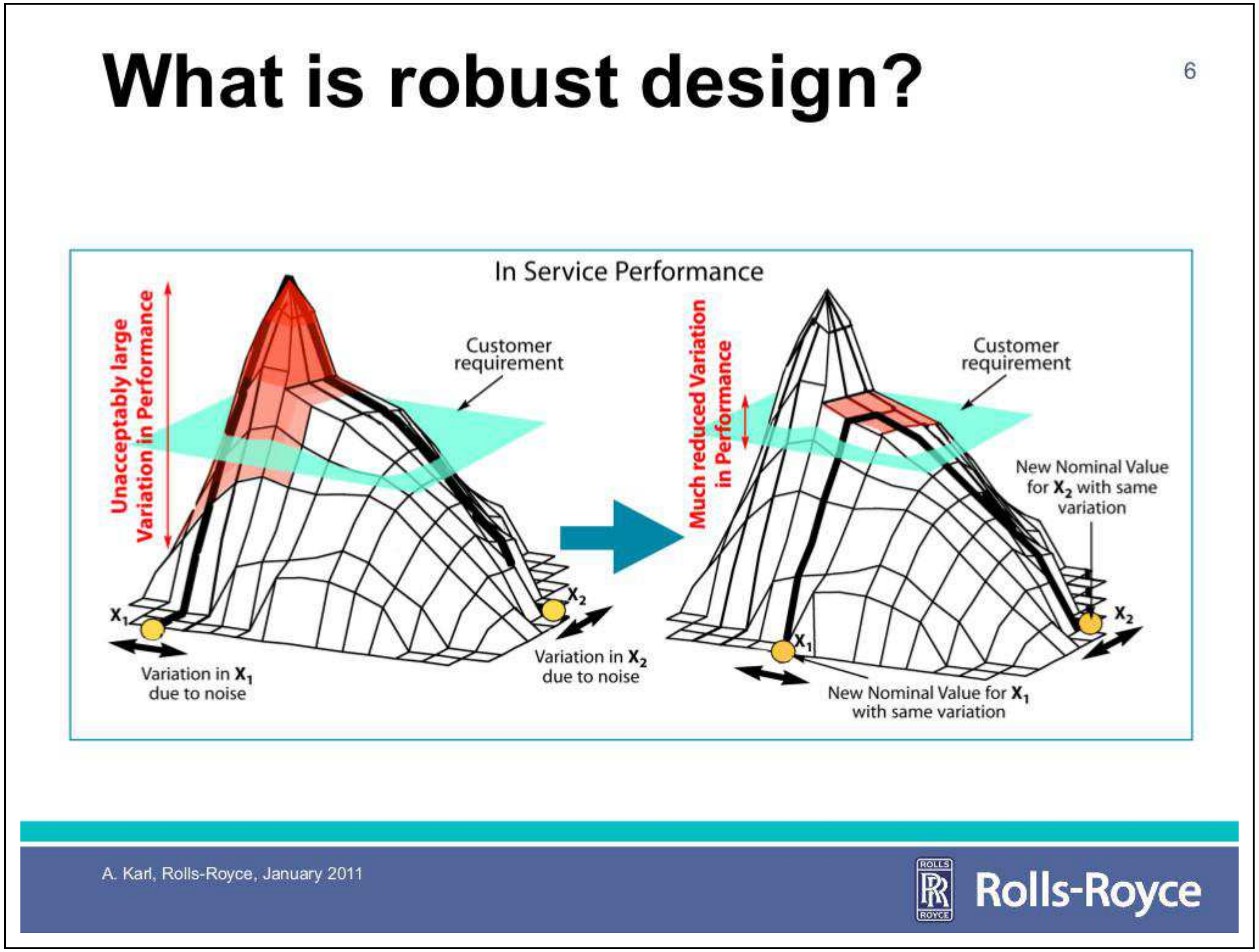
Example: Robust design and optimization in aerospace and mechanical engineering



From: A. Karl, B. Farris, L. Brown, and N. Metzger (Rolls-Royce). Robust design and optimization: Key methods and applications. Stanford, 2011.

Motivation

Example: Manufacturing tolerances in metal forming processes

Raw materials variability:
- Material properties.

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Process variability:
- Blank holder force.
- Initial dimensions.
- Friction.

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Modeling limitations:
- Constitutive model.
- FE discretization.

. . .

Input variables.

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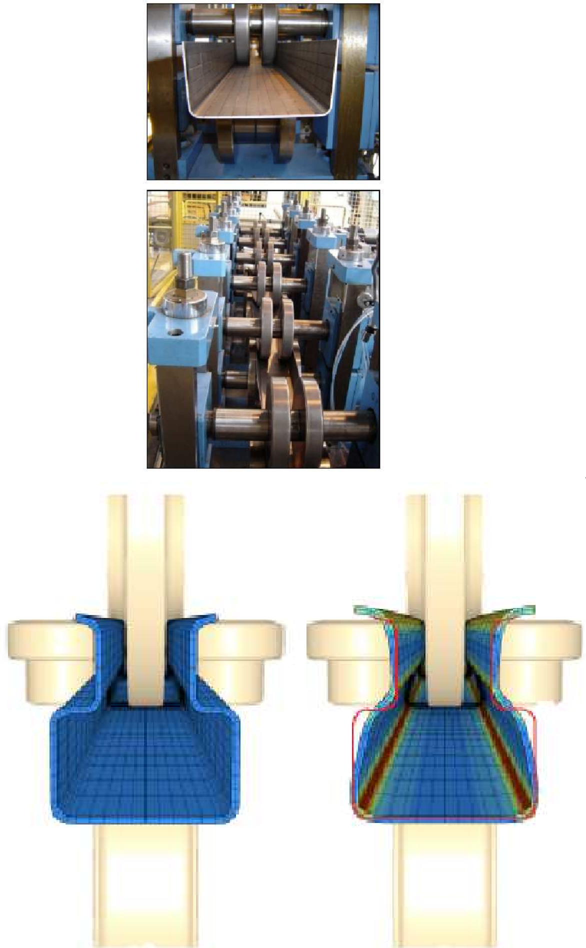

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Product variability:
- Final dimensions.
- Springback.

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Prediction limitations:
- Numerical noise.

. . .

Output variables.

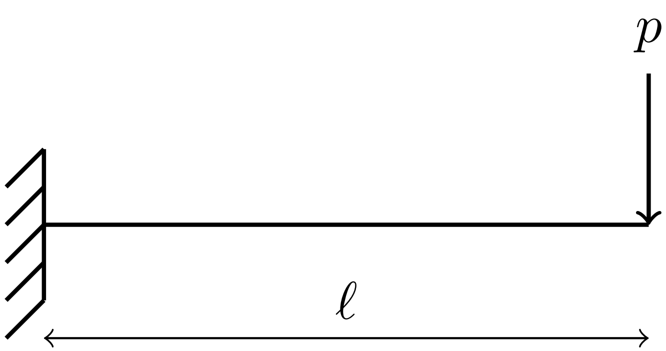
From: M. Arnst and J.-P. Ponthot. Characterization, propagation, and management of uncertainties in metal forming applications. COMPLAS, Barcelona, Spain, 2013.

Outline

- Motivation.
- Outline.
- Functions of random variables.
- ISO 98.
- References.

Functions of random variables

Motivating example: Bending of a clamped beam



$$u = \frac{p\ell^3}{3yj} \quad \text{with} \quad \begin{cases} u : \text{tip displacement,} \\ p : \text{tip load,} \\ \ell : \text{beam length,} \\ y : \text{Young's modulus,} \\ j : \text{moment of inertia.} \end{cases}$$

Let p, ℓ, y, and j be uncertain (e.g., imperfect knowledge at design time, imperfect manufacturing when compared to the design,...). Given a probabilistic characterization of p, ℓ, y, and j in terms of a probability distribution, what is the probability distribution of the tip displacement u?

Model problem

$$\underbrace{y}_{\text{output variable}} = \underbrace{g}_{\text{function}}(\underbrace{x}_{\text{input variable}}) \quad \text{with} \quad g : \mathbb{R} \to \mathbb{R}.$$

Let x be uncertain (e.g., imperfect knowledge at design time, imperfect manufacturing when compared to the design,...). Given a probabilistic characterization of the input variable x in terms of a probability distribution, what is the probability distribution of the output variable y?

Random variables with values in $\mathbb{R}$

- The **probability distribution** P_Z of a random variable Z with values in $\mathbb{R}$ is the function that associates to any meaningful subset $\mathcal{B}$ of $\mathbb{R}$ the probability that the value taken by Z is in $\mathcal{B}$, that is,
$$P_Z(\mathcal{B}) = P(Z \in \mathcal{B}).$$
The probability distribution takes values in $[0, 1]$ and is normalized in that $P_Z(\mathbb{R}) = 1$.
- The **probability density function** ρ_Z of a probability distribution P_Z with respect to dz, if it exists, is the function from $\mathbb{R}$ with values in $\mathbb{R}^+$ such that for any meaningful subset $\mathcal{B}$ of $\mathbb{R}$, we have
$$P_Z(\mathcal{B}) = \int_{\mathcal{B}} \rho_Z(z)dz.$$
The probability density function is normalized in that $P_Z(\mathbb{R}) = \int_{\mathbb{R}} \rho_Z(z)dz = 1$.
- The **cumulative distribution function** c_Z of a random variable Z with probability distribution P_Z and probability density function ρ_Z is the function c_Z from $\mathbb{R}$ with values in $[0, 1]$ such that
$$c_Z(z) = P_Z(] - \infty, z]) = \int_{-\infty}^{z} \rho_Z(\tilde{z})d\tilde{z}.$$
The cumulative distribution function is nondecreasing and satisfies $\lim_{z\to-\infty} = 0$ and $\lim_{z\to+\infty} = 1$. By Leibniz's formula, the cumulative distribution function c_Z is related to the probability density function ρ_Z as follows:
$$\frac{dc_Z}{dz}(z) = \rho_Z(z).$$

Random variables with values in $\mathbb{R}$ (continued)

- The **characteristic function** ϕ_Z of a random variable Z with PDF ρ_Z is the inverse Fourier transform of this PDF ρ_Z:
$$\phi_Z(\xi) = \frac{1}{2\pi} E\big(\exp(i\xi Z)\big) = \frac{1}{2\pi} \int_{\mathbb{R}} \exp(i\xi z)\rho_Z(z)dz \quad \text{with} \quad \phi_Z : \mathbb{R} \to \mathbb{C}.$$
Because the PDF ρ_Z is integrable, the characteristic function ϕ_Z is continuous and bounded.

- A random variable Z with PDF ρ_Z is of the **second order** if
$$E(Z^2) = \int_{\mathbb{R}} z^2 \rho_Z(z)dz < +\infty.$$

  The **mean** $\overline{z}$ of a second-order random variable Z with PDF ρ_Z is defined by
$$\overline{z} = E(Z) = \int_{\mathbb{R}} z\rho_Z(z)dz.$$

  The **variance** σ_Z^2 of a second-order random variable Z with PDF ρ_Z is defined by
$$\sigma_Z^2 = E\big((Z-\overline{z})^2\big) = \int_{\mathbb{R}} (z-\overline{z})^2 \rho_Z(z)dz.$$
  We have $\sigma_Z^2 = E\big((Z-\overline{z})^2\big) = E(Z^2) - \overline{z}^2$.

Random variables with values in $\mathbb{R}$ (continued)

- For example, a random variable Z with values in $\mathbb{R}$ is a **Gaussian** random variable with mean $\overline{z}$ and variance σ_Z^2 if it admits the probability density function

$$\rho_Z(z) = \frac{1}{\sqrt{2\pi}\sigma_Z} \exp\left(-\frac{(z-\overline{z})^2}{2\sigma_Z^2}\right).$$

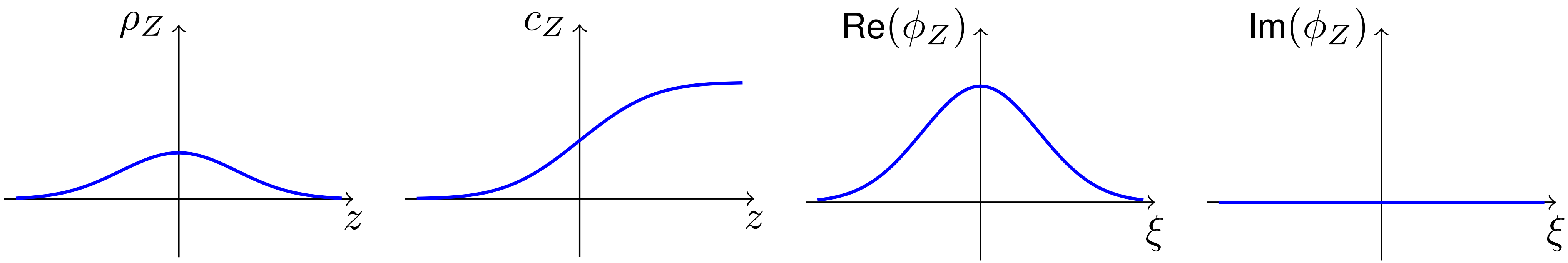
The corresponding cumulative distribution function reads as

$$c_Z(z) = \int_{-\infty}^{z} \frac{1}{\sqrt{2\pi}\sigma_Z} \exp\left(-\frac{(\tilde{z}-\overline{z})^2}{2\sigma_Z^2}\right) d\tilde{z}.$$

And the corresponding characteristic function reads as

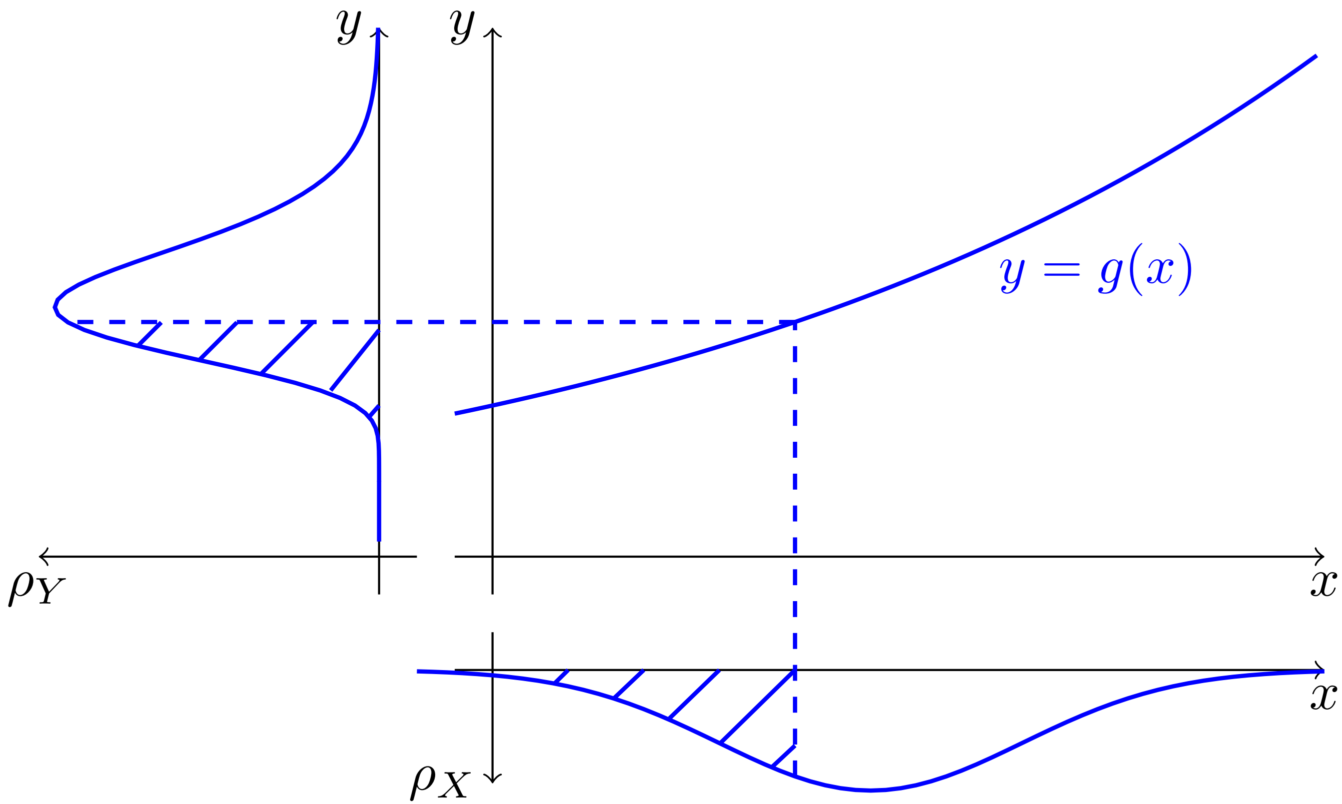
$$\phi_Z(\xi) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} \exp(i\xi z) \frac{1}{\sqrt{2\pi}\sigma_Z} \exp\left(-\frac{(\tilde{z}-\overline{z})^2}{2\sigma_Z^2}\right) d\tilde{z} = \exp\left(i\overline{z}\xi - \frac{1}{2}\sigma_Z^2\xi^2\right).$$

A Gaussian r.v. Z with $\overline{z} = 0$ and $\sigma_Z = 1$ is called a standard Gaussian r.v. The PDF, the CDF, and the characteristic function of a standard Gaussian r.v. take the following form:



Case of strictly increasing function

- If the function g is strictly increasing, we can establish the following **relationship between the cumulative distribution functions** c_X and c_Y of the input and output variables:



$$P\big(Y \leq y\big) = P\big(X \leq g^{-1}(y)\big) \quad \text{hence} \quad c_Y\big(y\big) = c_X\big(g^{-1}(y)\big).$$

Case of strictly increasing function (continued)

- If c_X, c_Y, and g are differentiable, using the chain rule, we can deduce the following **relationship between the probability density functions** ρ_X and ρ_Y of the input and output variables:

$$\frac{dc_Y}{dy}(y) = \frac{dc_X}{dx}\left(g^{-1}(y)\right)\frac{dg^{-1}}{dy}(y) \quad \text{hence} \quad \rho_Y(y) = \rho_X\left(g^{-1}(y)\right)\left(\frac{dg}{dx}\left(g^{-1}(y)\right)\right)^{-1}.$$

- Using the change-of-variables formula, we can deduce the following **relationship between the probability distributions** P_X and P_Y of the input and output variables:

$$P_Y(\mathcal{B}) = \int_{\mathcal{B}} \rho_Y(y)dy = \int_{\mathcal{B}} \rho_X\left(g^{-1}(y)\right)\left(\frac{dg}{dx}\left(g^{-1}(y)\right)\right)^{-1} dy$$

$$= \int_{g^{-1}(\mathcal{B})} \rho_X(x)\left(\frac{dg}{dx}(x)\right)^{-1}\frac{dg}{dx}(x)dx = \int_{g^{-1}(\mathcal{B})} \rho_X(x)dx = P_X\left(g^{-1}(\mathcal{B})\right).$$

- For example, if the input variable has the **Gaussian** probability density function

$$\rho_X(x) = \frac{1}{\sqrt{2\pi}\sigma_X}\exp\left(-\frac{(x-\overline{x})^2}{2\sigma_X^2}\right)$$

  and the function is the **exponential function**

$$y = g(x) = \exp(x),$$

  then the output variable has the following **lognormal** probability density function:

$$\rho_Y(y) = \frac{1}{\sqrt{2\pi}\sigma_X}\exp\left(-\frac{(\log(y)-\overline{x})^2}{2\sigma_X^2}\right)\frac{1}{y}.$$

Case of strictly increasing function (continued)

- Provided that the output variable is of the second order, using the change-of-variables formula, we can deduce the following expression for the **mean** $\overline{y}$:

$$\overline{y} = \int_{\mathbb{R}} y \rho_Y(y) dy = \int_{\mathbb{R}} y \rho_X\left(g^{-1}(y)\right) \left(\frac{dg}{dx}\left(g^{-1}(y)\right)\right)^{-1} dy$$
$$= \int_{\mathbb{R}} g(x)\rho_X(x) \left(\frac{dg}{dx}(x)\right)^{-1} \frac{dg}{dx}(x) dx = \int_{\mathbb{R}} g(x)\rho_X(x) dx,$$

and we can deduce the following expression for the **variance** σ_Y^2:

$$\sigma_Y^2 = \int_{\mathbb{R}} (y-\overline{y})^2 \rho_Y(y) dy = \int_{\mathbb{R}} (y-\overline{y})^2 \rho_X\left(g^{-1}(y)\right) \left(\frac{dg}{dx}\left(g^{-1}(y)\right)\right)^{-1} dy$$
$$= \int_{\mathbb{R}} (g(x)-\overline{y})^2 \rho_X(x) \left(\frac{dg}{dx}(x)\right)^{-1} \frac{dg}{dx}(x) dx = \int_{\mathbb{R}} (g(x)-\overline{y})^2 \rho_X(x) dx.$$

- Similarly, we can deduce the following expression for the **characteristic function** ϕ_Y:

$$\phi_Y(\xi) = \frac{1}{2\pi} \int_{\mathbb{R}} \exp(i\xi y) \rho_Y(y) dy = \int_{\mathbb{R}} \exp(i\xi y) \rho_X\left(g^{-1}(y)\right) \left(\frac{dg}{dx}\left(g^{-1}(y)\right)\right)^{-1} dy$$
$$= \int_{\mathbb{R}} \exp\left(i\xi g(x)\right) \rho_X(x) \left(\frac{dg}{dx}(x)\right)^{-1} \frac{dg}{dx}(x) dx = \int_{\mathbb{R}} \exp\left(i\xi g(x)\right) \rho_X(x) dx.$$

Case of strictly increasing function (continued)

- If the function is an **affine function**, that is,

$$y = g(x) = ax + b \quad \text{with} \quad a \text{ and } b \text{ constants,}$$

then we can immediately apply the expressions obtained previously for a strictly increasing function if $a > 0$ and the extension of these expressions to a strictly decreasing function if $a < 0$.

We obtain the following expressions for the mean $\overline{y}$:

$$\overline{y} = \int_{\mathbb{R}} y\rho_Y(y)dy = \int_{\mathbb{R}} (ax + b)\rho_X(x)dx = a\int_{\mathbb{R}} x\rho_X(x)dx + b\int_{\mathbb{R}} \rho_X(x)dx = a\overline{x} + b.$$

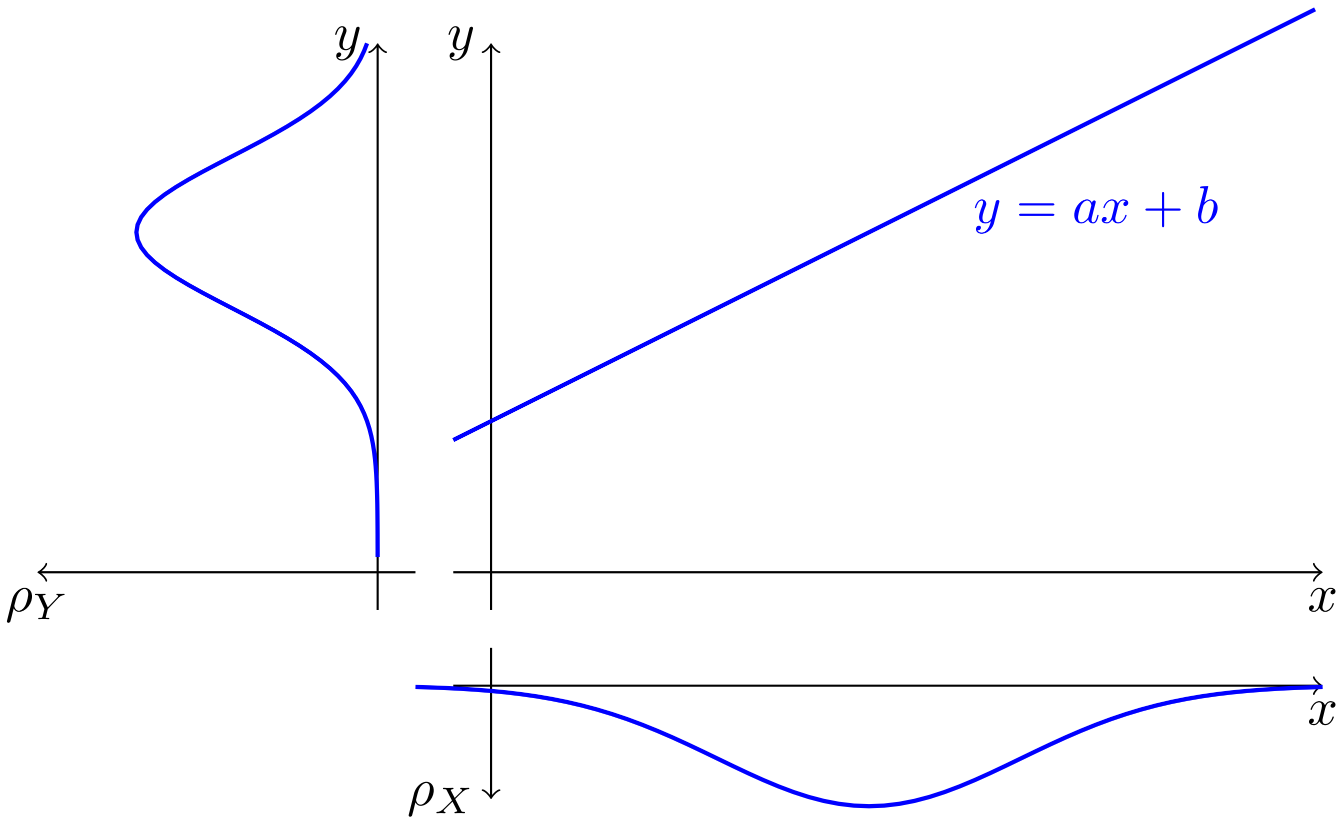
We obtain the following expressions for the variance σ_Y^2:

$$\sigma_Y^2 = \int_{\mathbb{R}} (y-\overline{y})^2\rho_Y(y)dy = \int_{\mathbb{R}} \big(ax+b-(a\overline{x}+b)\big)^2\rho_X(x)dx = a^2\int_{\mathbb{R}} (x-\overline{x})^2\rho_X(x)dx = a^2\sigma_X^2.$$

In conclusion, for a transformation through an affine function, knowledge of the mean and variance of the input variable suffices to determine the mean and variance of the output variable.

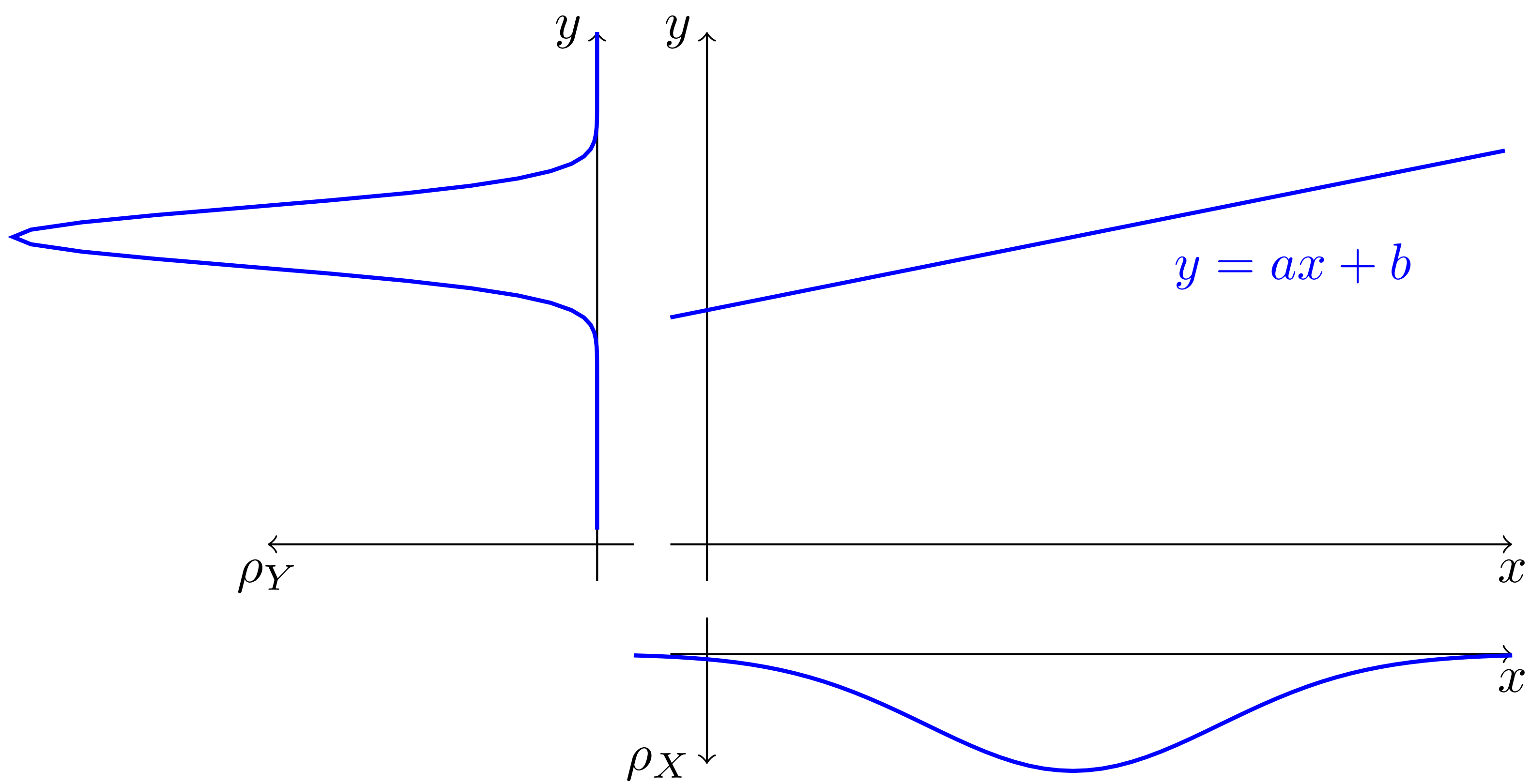
Case of strictly increasing function (continued)

- For example, affine function with stronger slope:



Case of strictly increasing function (continued)

- For example, affine function with weaker slope:



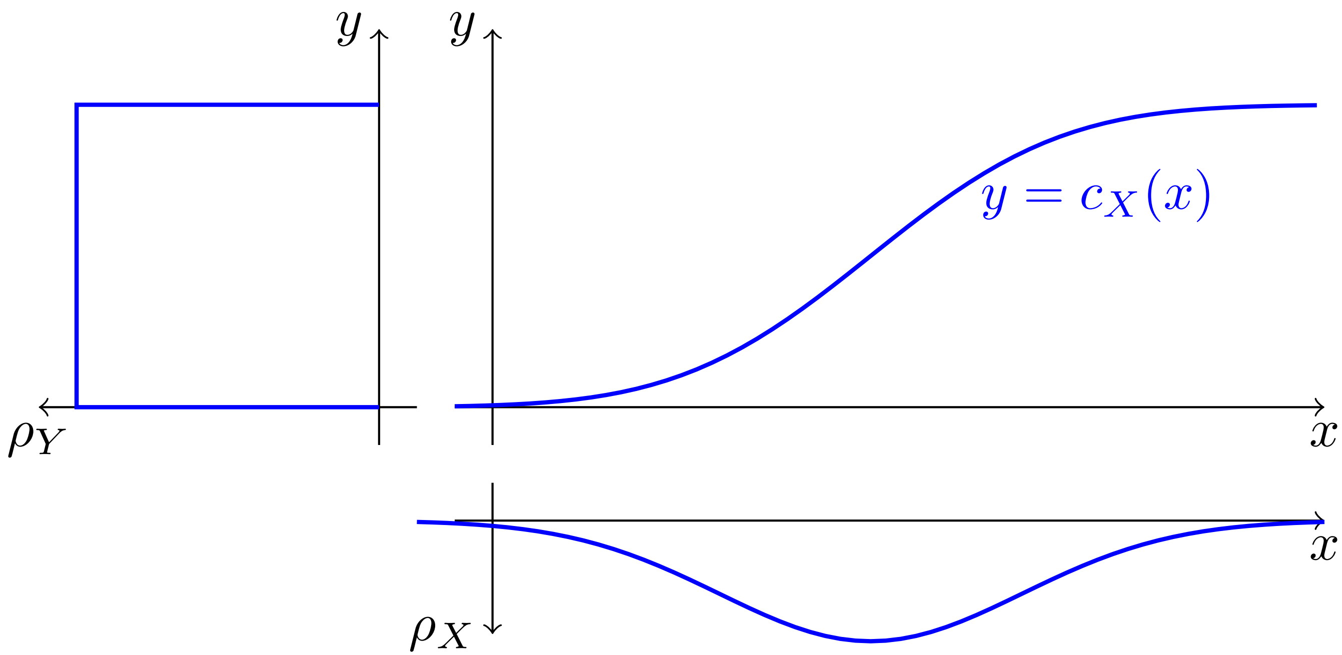
Case of strictly increasing function (continued)

- If the function is the cumulative distribution function of the input variable,

$$y = g(x) = c_X(x),$$

we obtain

$$\rho_Y(y) = \rho_X\big(c_X^{-1}(y)\big)\left(\frac{dc_X}{dx}\big(c_X^{-1}(y)\big)\right)^{-1} = \rho_X\big(c_X^{-1}(y)\big)\rho_X\big(c_X^{-1}(y)\big)^{-1} = 1.$$



Thus, the transformation of a random variable through its own cumulative distribution function results in a uniform random variable with values in the interval $[0, 1]$. This result is known in probability theory as the **isoprobability transform**.

Case of general function

- For a general function g, where we mean by "general" that this function is not necessarily strictly increasing, probability theory still allows to establish a relationship between the probability distributions P_X and P_Y of the input and output variables:
$$P_Y\big(\mathcal{B}\big) = P_X\big(\{x \in \mathbb{R} \;:\; g(x) \in \mathcal{B}\}\big).$$
However, whereas we were able to establish explicit relationships between the probability density functions ρ_X and ρ_Y and between the cumulative distribution functions c_X and c_Y for a strictly increasing function g, we cannot in general obtain such explicit relationships for a general function g.

- For a general function g, probability theory provides a change-of-variables theorem that asserts that
$$\int_{\mathbb{R}} h(y) P_Y\big(dy\big) = \int_{\mathbb{R}} h\big(g(x)\big) P_X\big(dx\big),$$
that is, if P_X and P_Y admit PDFs ρ_X and ρ_Y,
$$\int_{\mathbb{R}} h\big(y\big)\rho_Y\big(y\big)dy = \int_{\mathbb{R}} h\big(g(x)\big)\rho_X\big(x\big)dx,$$
for any integrand h for which either integral exists. This formula is consistent with the change-of-variables formulas applied previously in our study of the case of a strictly increasing function g.

- A detailed treatment of the case of a general function requires recourse to measure and probability theory. For details, please refer, for example, to [Dudley, 2002] or [Wehenkel, 2013].

Case of general function (continued)

- Provided that the output variable is of the second order, using the change-of-variables formula, we can deduce the following expression for the **mean** $\overline{y}$:

$$\overline{y} = \int_{\mathbb{R}} y P_Y(dy) = \int_{\mathbb{R}} g(x) P_X(dx), \text{ that is, if } P_X \text{ admits PDF } \rho_X, \ \overline{y} = \int_{\mathbb{R}} g(x)\rho_X(x)dx,$$

and we can deduce the following expression for the **variance** σ_Y^2:

$$\sigma_Y^2 = \int_{\mathbb{R}} (y - \overline{y})^2 P_Y(dy) = \int_{\mathbb{R}} \big(g(x) - \overline{y}\big)^2 P_X(dx), \text{ that is, if } P_X \text{ admits PDF } \rho_X, \ \sigma_Y^2 = \int_{\mathbb{R}} \big(g(x) - \overline{y}\big)^2 \rho_X(x)dx.$$

In conclusion, for a transformation through a general function, knowledge of the mean and variance of the input variable does not suffice to determine the mean and variance of the output variable! Knowledge of the probability distribution of the input variable is required!

- Similarly, we can deduce the following expression for the **characteristic function** ϕ_Y:

$$\phi_Y(\xi) = \int_{\mathbb{R}} \exp(i\xi y) P_Y(dy) = \int_{\mathbb{R}} \exp\big(i\xi g(x)\big) P_X(dx), \text{ that is, if } P_X \text{ admits PDF } \rho_X, \ \phi_Y(\xi) = \int_{\mathbb{R}} \exp\big(i\xi g(x)\big)\rho_X(x)dx$$

ISO 98

GUIDE 98-3

Uncertainty of measurement —

Part 3:
Guide to the expression of uncertainty in measurement (GUM:1995)

Incertitude de mesure —

Partie 3: Guide pour l'expression de l'incertitude de mesure (GUM:1995)

ISO 98: Guide to the expression of uncertainty in measurement.

Introduction

- ISO 98 states that when reporting a measurement, it is obligatory that some quantitative indication of the quality of the result be given so that those who use it can assess its reliability.

  Without such an indication, measurement results cannot be compared, either among themselves or with reference values given in a specification or standard.

  It is therefore necessary that there be a readily implemented, easily understood, and generally accepted procedure for characterizing the quality of a result of a measurement, that is, for evaluating and expressing its uncertainty.

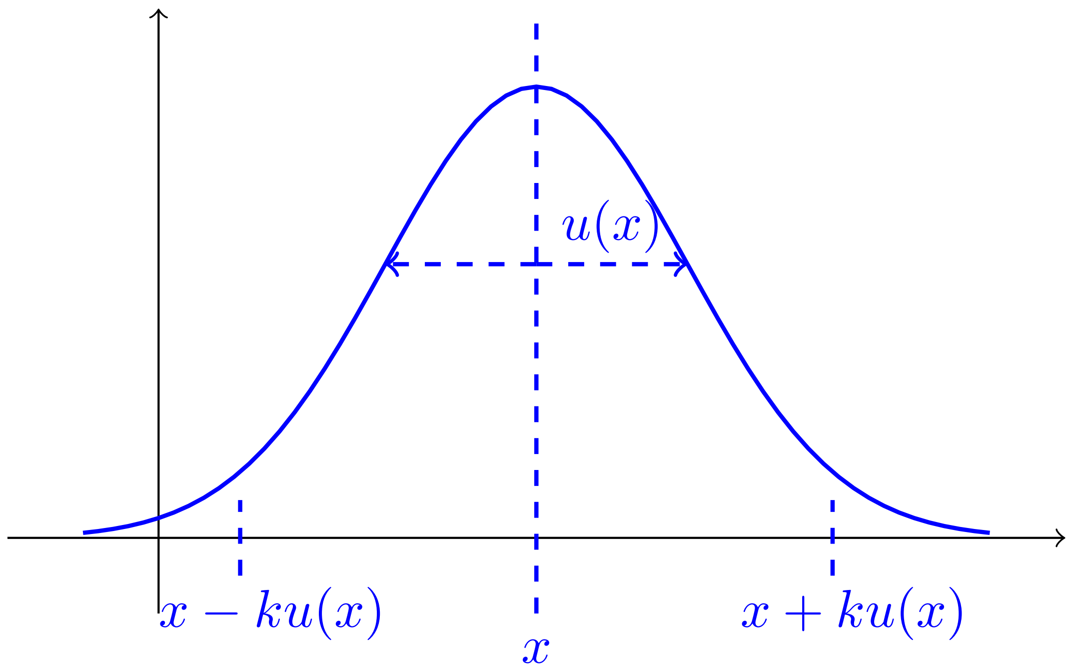
- ISO 98 states that the ideal method for evaluating and expressing uncertainty should be:
  - universal,
  - internally consistent,
  - transferable.

Definitions and basic concepts

- **Measurable quantity:** attribute of a phenomenon, body, or substance that may be distinguished qualitatively and determined quantitatively.
- **Measurand:** particular quantity subject to measurement.
- **Measurement value:** value attributed to a measurand, obtained by measurement.
- **Standard uncertainty:** uncertainty of the result of a measurement expressed as a standard deviation.
- **Expanded uncertainty:** quantity defining an interval about the result of a measurement that may be expected to encompass a large fraction of the distribution of values that could reasonably be attributed to the measurand.
- **Random error:** random error arises from unpredictable or stochastic temporal and spatial variations of influence quantities. The effects of such variations, termed random effects, give rise to variations in repeated observations of the measurand.
- **Systematic error:** systematic error arises from a recognized effect of an influence quantity on a measurement result.
- **Uncertainty of a measurement:** the uncertainty reflects the lack of knowledge of the value of the measurand due to random effects and from imperfect correction of the result for systematic effects.

Evaluating standard uncertainty

- ISO 98 is concerned with scalar uncertain quantities.
- ISO 98 uses the following descriptors of uncertainty:



- "best available estimate" x (we can make a link with mean value),
- "standard uncertainty" $u(x)$ (we can make a link with standard deviation),
- "expanded uncertainty" $x \pm U$ with $U = ku(x)$ (we can make a link with confidence interval).

Evaluating standard uncertainty (continued)

- As ISO 98 sees it, in most cases, a measurand is not measured directly, but is determined from other quantities through a functional relationship:
$$Y = g(X_1, X_2, \ldots, X_N),$$
in which $X_1, X_2, \ldots, X_N$ are input variables upon which the output variable Y depends.
- To obtain a best available estimate y and a standard uncertainty $u_c(y)$ associated with the output variable from best estimates x_1, x_2,..., x_N and standard uncertainties $u_c(x_1)$, $u_c(x_2)$,..., $u_c(x_N)$ associated with the input variables, ISO 98 proposes to proceed as follows:
$$y = g(x_1, x_2, \ldots, x_N),$$
$$\left(u_c(y)\right)^2 = \sum_{k=1}^{N} \left(\frac{dg}{dX}(x_k)\right)^2 \left(u_c(x_k)\right)^2.$$
We can interpret these formulas as the ones that probability theory would provide for determining the mean and standard deviation of the output variable from the mean values and standard deviations of the input variables if the function g was approximated by a first-order Taylor series
$$Y = g(X_1, X_2, \ldots, X_N) \approx g(x_1, x_2, \ldots, x_N) + \sum_{k=1}^{N} \left(\frac{dg}{dX}(x_k)\right)(X_k - x_k).$$
- Please note that ISO 98 also includes extensions of these formulas to the case wherein one may want to account for dependence among the input variables.

Evaluating standard uncertainty (continued)

- ISO 98 distinguishes between type A and type B methods for obtaining best available estimates and standard uncertainties associated with input variables.

- **Type A evaluation of uncertainty** is based on the statistical analysis of series of observations.

  To obtain a best available estimate of a quantity which varies randomly and for which n independent observations $x_1, \ldots, x_n$ have been obtained under the same conditions of measurement, ISO 98 proposes to use the arithmetic mean or avarage of these n independent observations:

$$x = \frac{1}{n} \sum_{k=1}^{n} x_k.$$

  To obtain a standard uncertainty associated with this best available estimate, ISO 98 proposes:

$$\big(u_c(x_k)\big)^2 = \frac{s^2(x)}{n} \quad \text{with} \quad s^2(x) = \frac{1}{n-1} \sum_{k=1}^{n} (x_k - x)^2.$$

  We can interpret these formulas in terms of the ones that probability theory would provide for the unbiased estimate of the mean, the variance of the unbiased estimator of the mean, and the unbiased estimate of the variance, respectively.

Evaluating standard uncertainty (continued)

- **Type B evaluation of uncertainty** is any evaluation by means other than the statistical analysis of series of observations.
- For an estimate of an input quantity that has not been obtained from repeated observations, the associated standard uncertainty can be evaluated by scientific judgement based on all of the available information on the possible variability. The pool of information may include:
  - previous measurement data,
  - experience with or general knowledge of the behaviour and properties of relevant materials and instruments,
  - manufacturer specifications,
  - data provided in calibration and other certificates,
  - uncertainties assigned to reference data taken from handbooks,
  - . . .
- Information may be provided in the form of:
  - expanded uncertainty without the associated coverage factor,
  - expanded uncertainty with the associated coverage factor,
  - probability density function,
  - . . .

Evaluating expanded uncertainty

- The expanded uncertainty U is obtained by multiplying the standard uncertainty $u_c(y)$ by a **coverage factor** k:

$$U = ku_{\mathrm{c}}(y).$$

- The result of a measurement is then conveniently expressed as $Y = y \pm U$, which ISO 98 interprets as meaning that the best estimate of the value attributed to the measurand is y and that $y - U$ to $y + U$ is an interval that may be expected to encompass a large fraction of the distribution of values that could reasonably be attributed to the measurand.

- ISO 98 bases the choice of the coverage factor on the basis of sampling distributions.

Reporting uncertainty

- When reporting the result of a measurement, and when the measure of uncertainty is the standard uncertainty, ISO 98 states that one should:
  - give a full description of how the measurand is defined,
  - give the best available estimate y of the measurand and its standard uncertainty $u_c(y)$; the units should always be given,
  - include the relative standard uncertainty $u_c(y)/y$, when appropriate.

- When reporting the result of a measurement, and when the measure of uncertainty is the expanded uncertainty $U = ku_c(y)$, one should:
  - give a full description of how the measurand is defined,
  - state the result of the measurement as $Y = y \pm U$ and give the units of y and U,
  - include the relative expanded uncertainty $U/|y|$, when appropriate,
  - give the value of k used to obtain U,
  - give the approximate level of confidence associated with the interval $Y = y \pm U$, and state how it was obtained.

Examples

- ISO 98 contains many examples that users can work through in preparation of putting the ISO 98 principles into practice in their own work:
  - end-gauge calibration,
  - simultaneous resistance and reactance measurement,
  - calibration of a thermometer,
  - measurement of activity,
  - analysis of variance,
  - measurement on a reference scale.

References

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