Modelling, Uncertainty and Data for Engineers (MUDE)

Week 1.6 : Uncertainty Propagation

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TU Delft

Welcome to...

MUDE

Modelling, Uncertainty, and Data for Engineers

WEEK 6!

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Background information

Learning Objectives

By the end of this week, you will be able

- To explain how uncertainty propagates through functions
- To apply (linear) propagation laws of mean and variances
- To adopt Monte Carlo simulations for propagating uncertainties

Motivation – Why shall we propagate the uncertainty?

Because for a given *stochastic* input of a certain transformation, also outputs will be *stochastic* but most likely with different characteristics, i.e. a different underlying distribution.

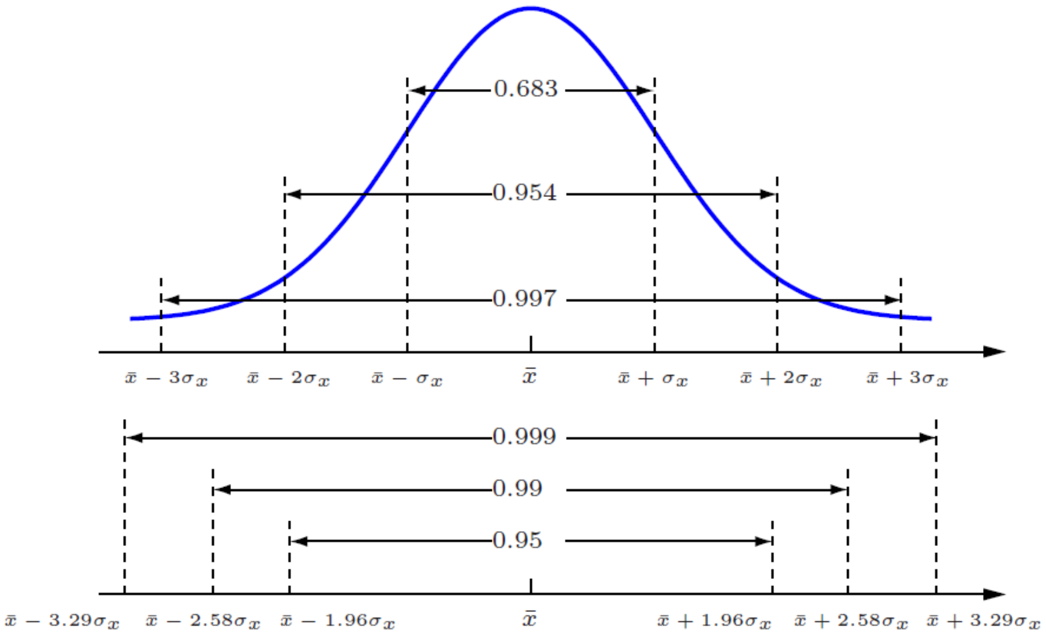
Content

1. Introduction
2. Transforming random variables
3. Mean and variance propagation laws
    1. …considering **linear** functions
    2. …considering **non-linear** functions
4. MC simulations for uncertainty propagation
5. Summary

Introduction

Small recap from Week 4 – Univariate distributions

A **univariate continuous distribution function** only takes a single variable as input, and so it assigns probability (densities) to this random variable.



Example of Gaussian PDF – see details in **ProbObs2009**

PDF = Probability Density Function

Small recap from Week 4 – Univariate distributions

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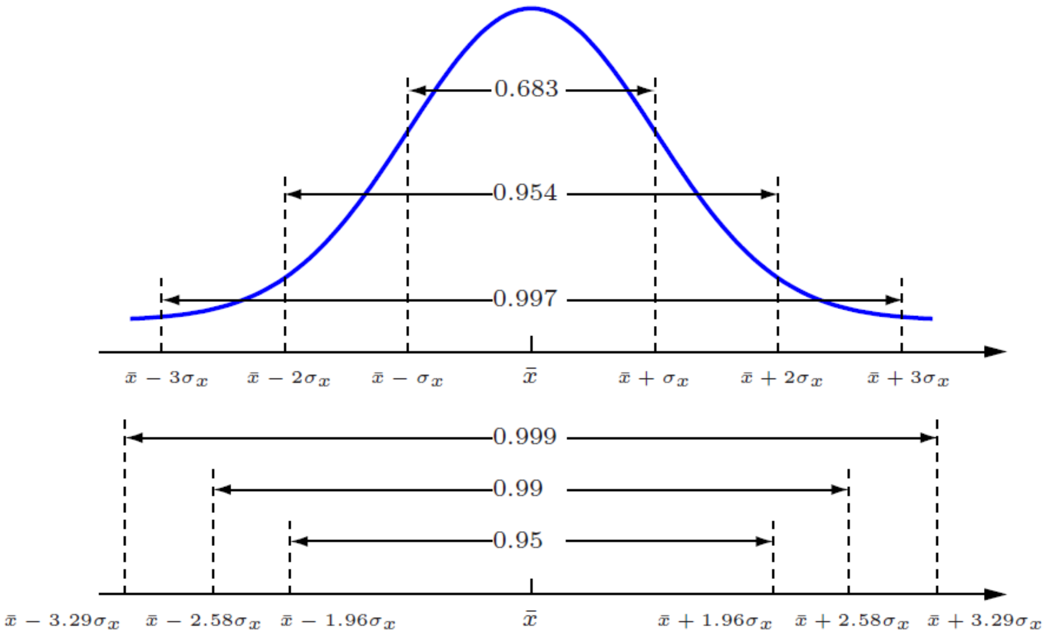


Example of Gaussian PDF – see details in **ProbObs2009**

PDF = Probability Density Function

Mean, variance and higher-order moments

If x is continuous with PDF being $f_x(x)$, then

Mean: $$E\{x\} \stackrel{\text{def}}{=} \bar{x} = \int_{-\infty}^{+\infty} x\, f_x(x)dx$$

Variance: $$Var\{x\} \stackrel{\text{def}}{=} \sigma^2 = \underbrace{\int_{-\infty}^{+\infty} (x - \bar{x})^2 f_x(x)dx}_{\equiv E\{(x-\bar{x})^2\}}$$

…

$$\mu_n = \int_{-\infty}^{+\infty} (x - \bar{x})^n f_x(x)dx$$

Small recap from Week 5 – Multivariate distributions

Joint probabilities

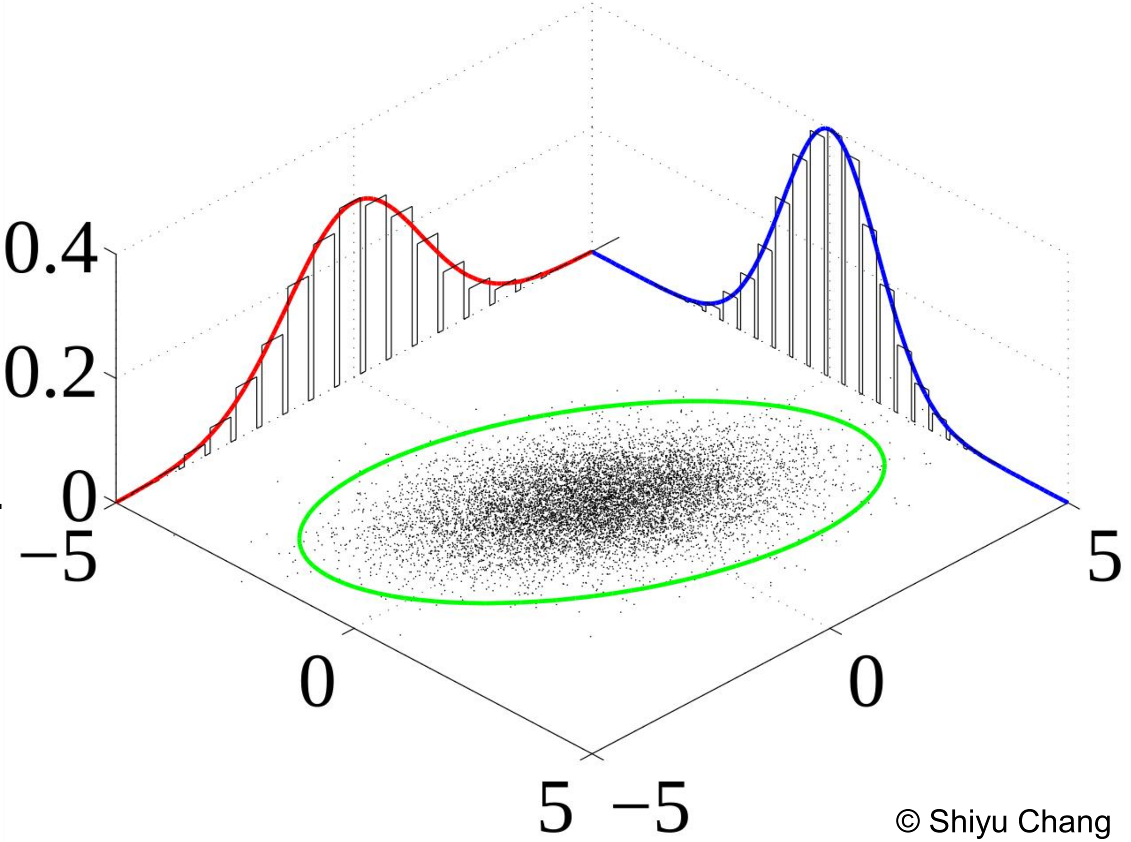
A probability distribution related to multiple random variables $\mathrm{X}, \mathrm{Y}, \ldots$, which can be independent or dependent. If variables are independent, then Pearson's correlation is zero!

Covariance $Cov(\mathrm{X}, \mathrm{Y})$:

- Measure of joint variability of two variables.

Pearson's coefficient ρ:

- Measure of linear correlation between two variables.



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Transforming random variables

Function inputs: deterministic vs stochastic

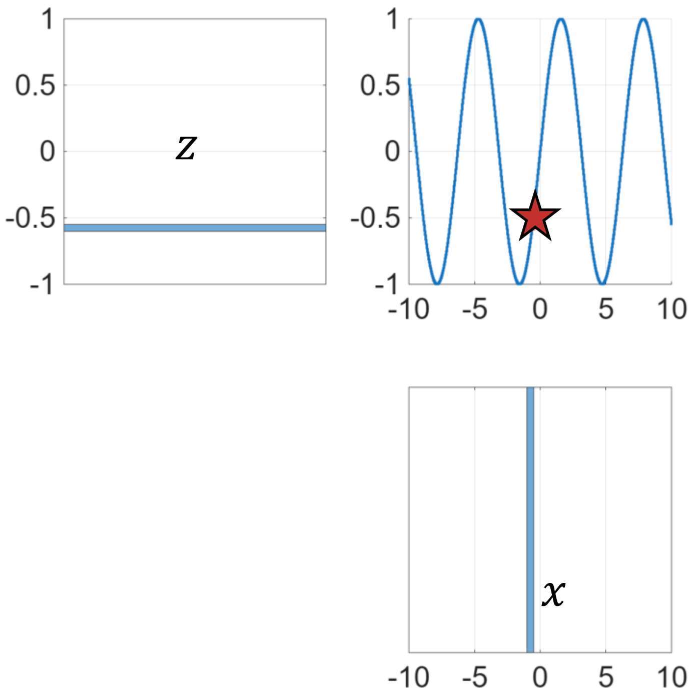
The function is

$$g(x) = \sin(\mathrm{x})$$

with $\mathrm{x} \sim \mathcal{N}(0, \sigma^2)$

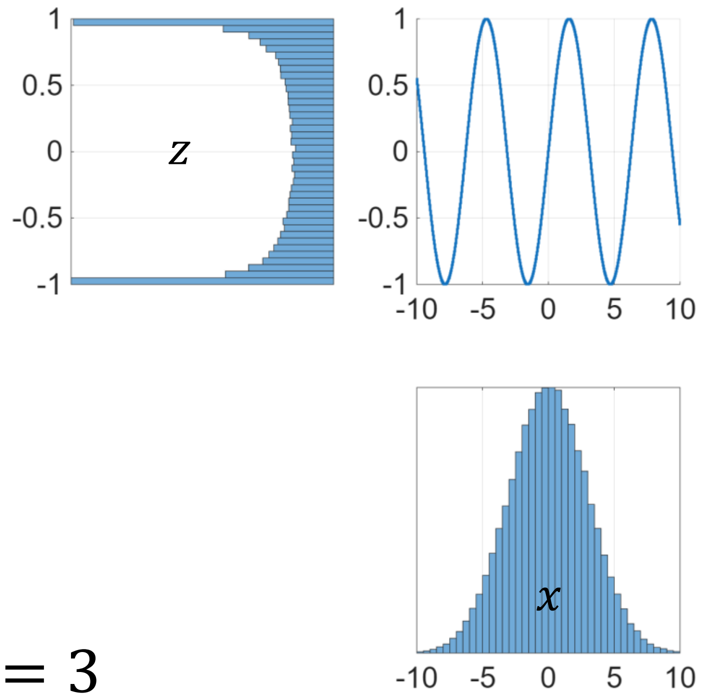
Deterministic case

We take $z = g(x)$, for x being *deterministic*.



Stochastic case

We take $z = g(x)$, for x being *random variable*.



Case $\sigma = 3$

Function inputs: deterministic vs stochastic

The function is

$$g(x) = \sin(x)$$

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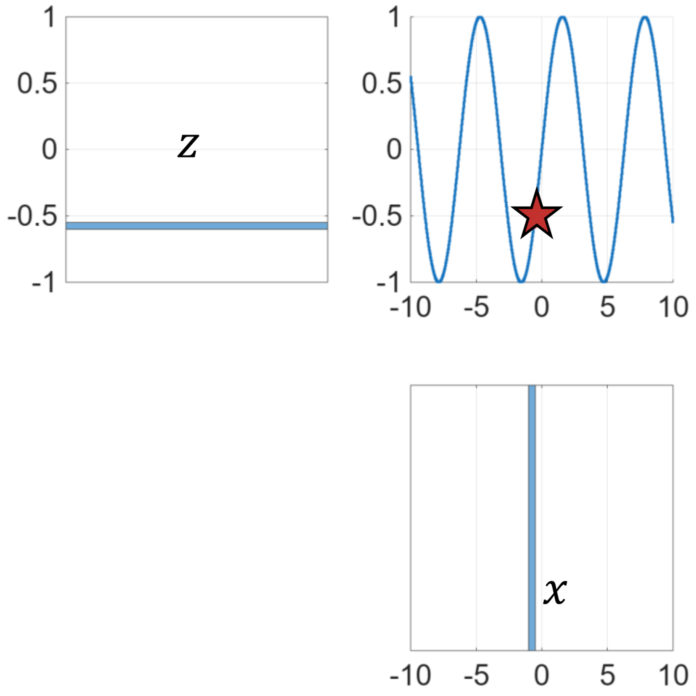
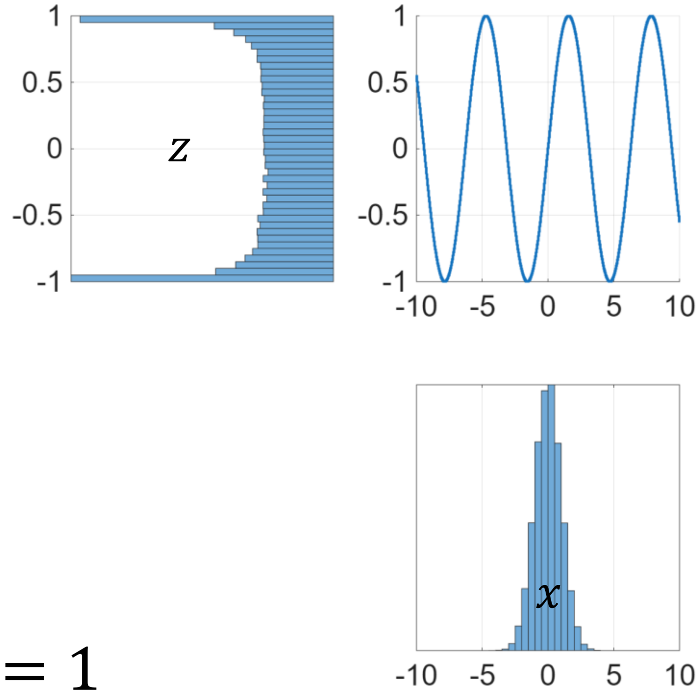


Stochastic case

We take $z = g(x)$, for x being *random variable*.



Case $\sigma = 1$

Function inputs: deterministic vs stochastic

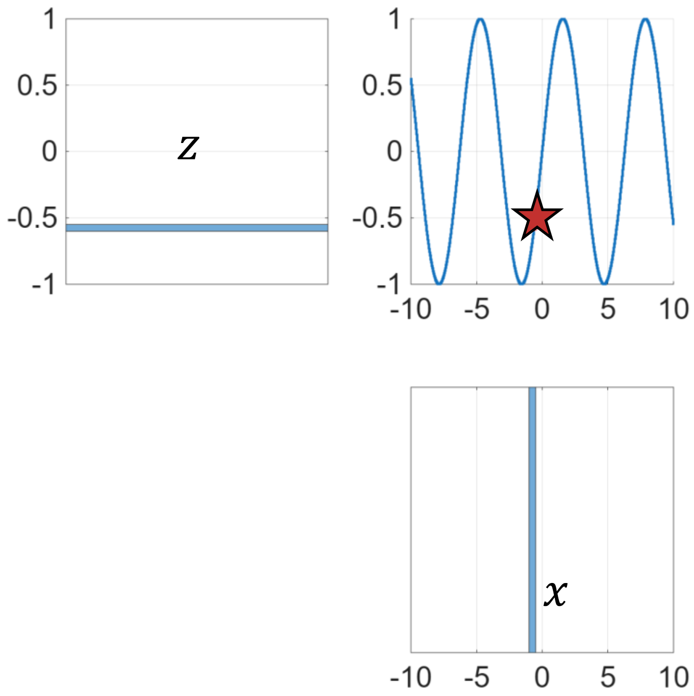
The function is

$$g(x) = \sin(\mathrm{x})$$

with $\mathrm{x} \sim \mathcal{N}(0, \sigma^2)$

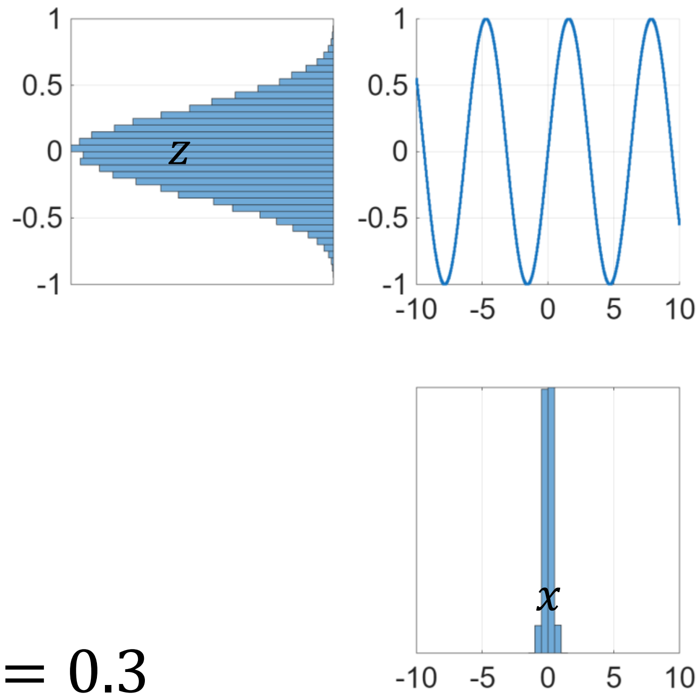
Deterministic case

We take $z = g(x)$, for x being *deterministic*.



Stochastic case

We take $z = g(x)$, for x being *random variable*.



Case $\sigma = 0.3$

Some examples from physical problems

- Temperature conversion from Celsius to Fahrenheit

  $T_f = q(T_c) = \frac{9}{5}T_c + 32$

- Compute the mean of m repeated measurements Y_i

  $\hat{X} = q(Y_1, \ldots, Y_m) = \frac{1}{m}\sum_{i=1}^{m} Y_i$ → Weeks 7 & 8!

- Subsurface temperature T_z as a function of depth Z and surface temperature T_0, given a known factor a

  $T_z = q(T_0, Z) = T_0 + a \cdot Z$

- Wind loading F on a building as function of area of building face A, wind pressure P, drag coefficient C

  $F = q(A, P, C) = A \cdot P \cdot C$

- Evaporation Q using Bowen Ratio Energy Balance as function of the net radiation R, ground heat flux G, bowen ratio B

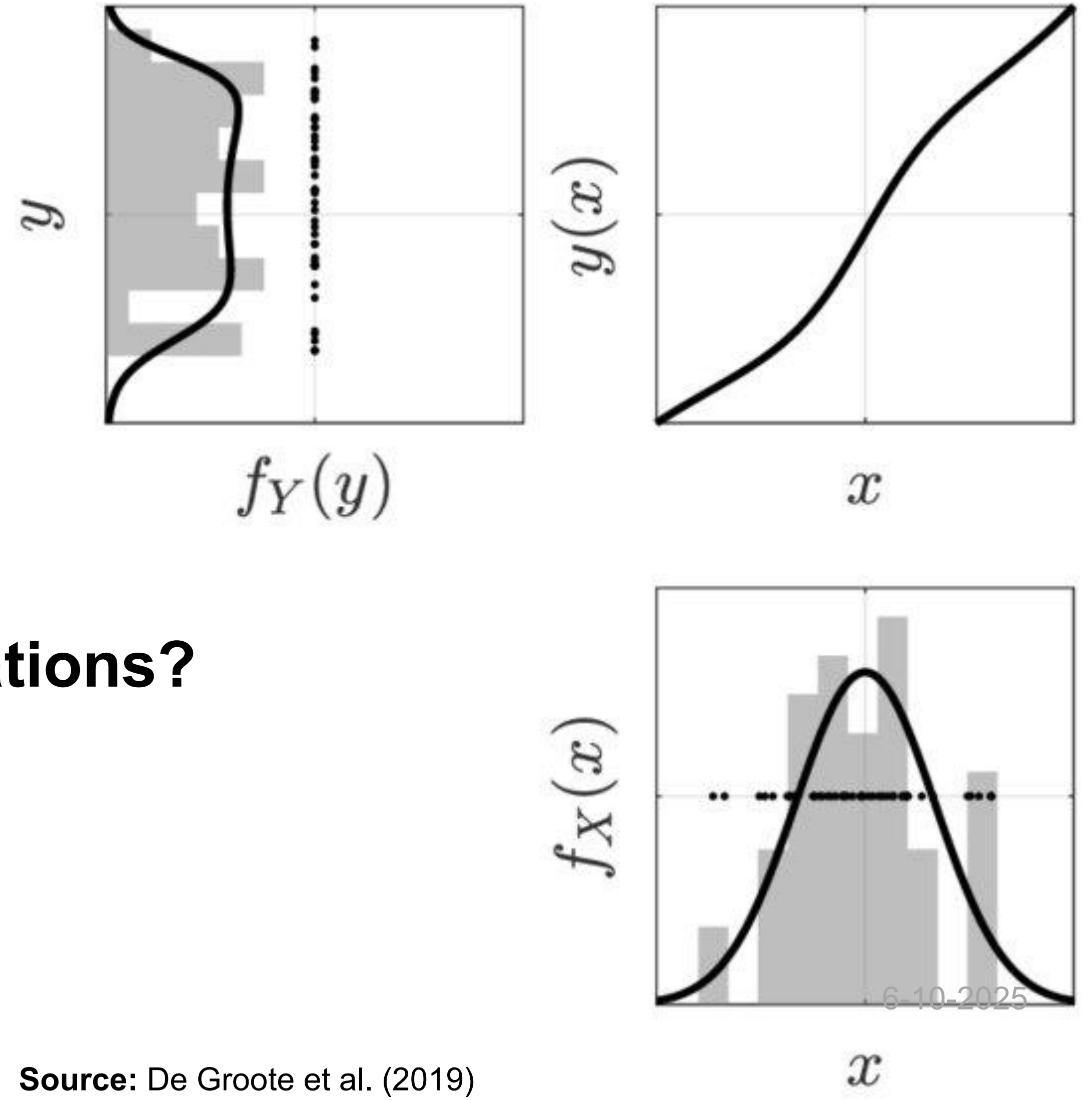
  $Q = q(R, G, B) = \frac{R-G}{1-B}$

What comes in, then shall come out

Generic transformations

Distributions of output variables might be often changed due to a non-linear transformation.

➢ **Therefore, their PDF & CDF will change!**



What about simpler linear transformations?

Let's see an illustrative example…

Source: De Groote et al. (2019)

Linear transformation

$$T_f \stackrel{\text{def}}{=} q(T_c) = \frac{9}{5} T_c + 32$$

Example: transformation of units

Temperature measurements are converted from degrees Celsius to Fahrenheit…

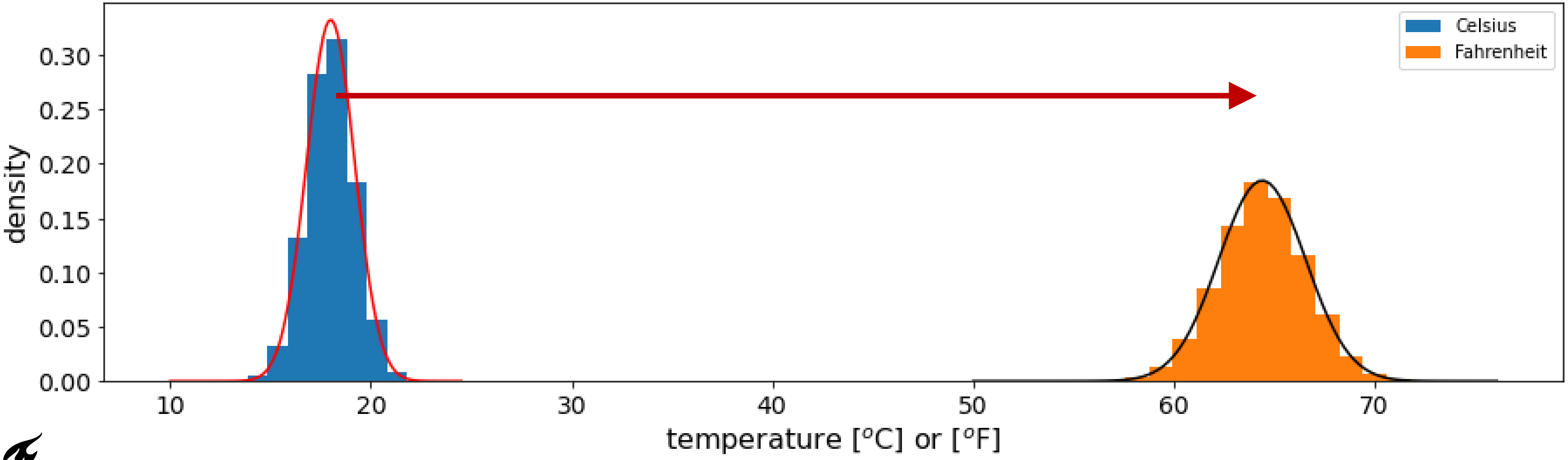
Linear transformation

$$T_f \stackrel{\text{def}}{=} q(T_c) = \frac{9}{5}T_c + 32$$

Example: transformation of units

Temperature measurements are converted from degrees Celsius to Fahrenheit…

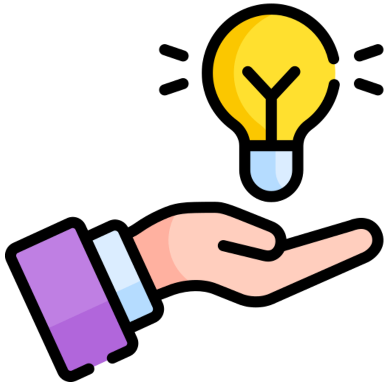
- **What do you notice? Why does the temperature in F° look less accurate?**



Generic CDF transformation of univariate functions

Given $Z = g(X)$, for a generic function g and random variable X, then its CDF is given by

$$F_Z(z) \underset{\text{Definition of CDF}}{=} P(Z \leq z) \underset{\text{Definition of } Z}{=} P(g(X) \leq z) \underset{\text{Definition of } I_z}{=} P(X \in I_z)$$



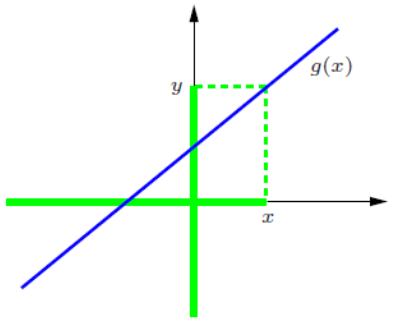
where $I_z = \{\mathrm{x} \in \mathbb{R} \mid \mathrm{g(x)} \leq \mathrm{z}\}$, i.e. all x values that satisfy $\mathrm{g(x)} \leq \mathrm{z}$ for a given z.

Workout example

Linear transformation: $z = g(x) = ax + b$

Any volunteer on the board?

Workout solution



Case $a > 0$

Linear transformation: $z = g(x) = ax + b$

We consider three cases:

- Case $a > 0$:

$$F_Z(z) = P(Z \leq z) = P(aX + b \leq z) = P\left(X \leq \frac{z-b}{a}\right) = F_X\left(\frac{z-b}{a}\right)$$

Workout solution

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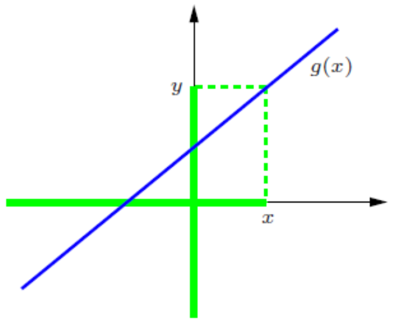

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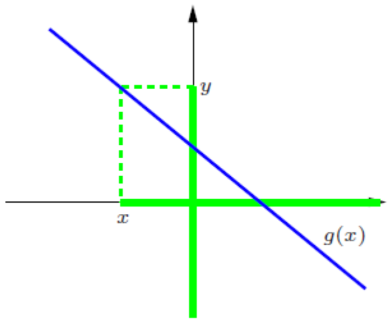

Case $a < 0$

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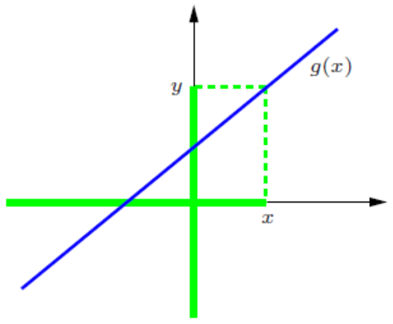
- Case $a < 0$:

$$F_Z(z) = P(Z \leq z) = P(aX + b \leq z) = P\left(X \geq \frac{z-b}{a}\right) = 1 - F_X\left(\frac{z-b}{a}\right)$$

Workout solution



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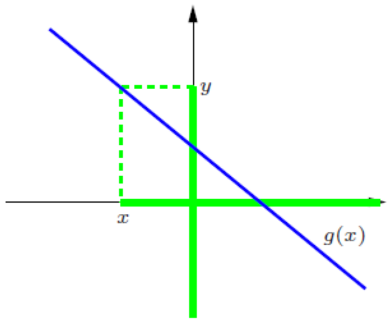

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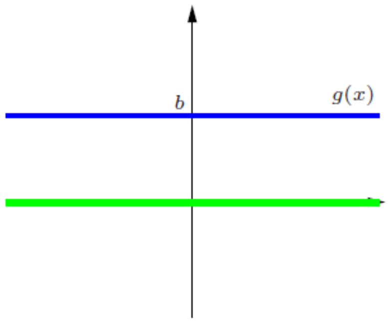

Case $a = 0$

Linear transformation: $z = g(x) = ax + b$

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$$F_Z(z) = P(Z \leq z) = P(a\mathrm{X} + b \leq z) = P\left(\mathrm{X} \leq \frac{z-b}{a}\right) = \boxed{F_X\left(\frac{z-b}{a}\right)}$$

It looks familiar…

- Case $a < 0$:

$$F_Z(z) = P(Z \leq z) = P(a\mathrm{X} + b \leq z) = P\left(\mathrm{X} \geq \frac{z-b}{a}\right) = 1 - F_X\left(\frac{z-b}{a}\right)$$

- Case $a = 0$:

$$F_Z(z) = P(Z \leq z) = \begin{cases} 1, & z \geq b \\ 0, & z < b \end{cases}$$

Expectation & Variance propagation laws

In general, computing CDF (or PDF) for arbitrary distribution and/or functions is cumbersome, therefore we might restrict ourselves to first two moments, i.e. Mean & Variance.

Theorem (Expectation law)

For $\mathbf{X} \in \mathbb{R}^n$ being an n-dimensional random vector with continuous PDF $f_{\mathbf{X}}(\mathbf{x})$, we consider $\mathbf{Z} = \mathbf{g}(\mathbf{X})$, where $\mathbf{g} : \mathbb{R}^n \to \mathbb{R}^m$ has continuous first partial derivatives. Then the expectation of $\mathbf{Z}$ is

$$\mathbb{E}(\mathbf{Z}) = \mathbb{E}(\mathbf{g}(\mathbf{X})) = \int_{\mathbb{R}^n} \mathbf{g}(x) f_{\mathbf{X}}(x) dx$$

Corollary (Variance law)

Under the same assumptions, the variance of $\mathbf{Z}$ is

$$\mathrm{Var}(\mathbf{Z}) = \mathrm{Var}(\mathbf{g}(\mathbf{X})) = \int_{\mathbb{R}^n} [\mathbf{g}(\mathbf{x}) - \boldsymbol{\mu}_z][\mathbf{g}(\mathbf{x}) - \boldsymbol{\mu}_z]^T f_{\mathbf{X}}(\mathbf{x}) d\mathbf{x}$$

where $\boldsymbol{\mu}_z = \mathbb{E}(\mathbf{g}(\mathbf{X}))$, which is described in the previous Theorem.

IMPORTANT NOTE
Proof is rather complicated and **not** treated in this course; <u>these expressions holds if</u>

I) Random vector with continuous PDF,

II) Continuous first partial derivatives.

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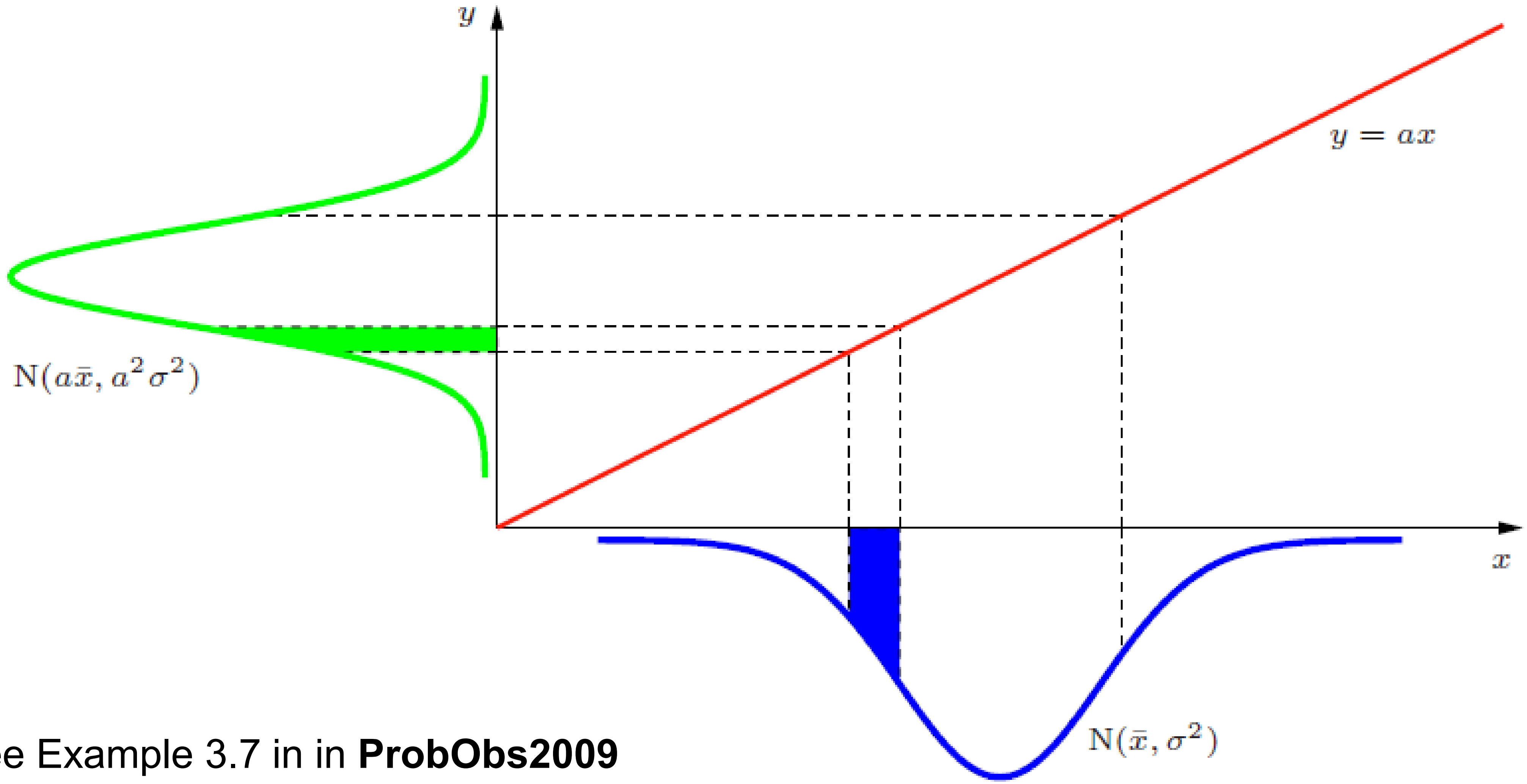
where $\boldsymbol{\mu}_z = \mathbb{E}(\mathbf{g}(\mathbf{X}))$, which is described in the previous Theorem.

Remember, if…	…X is Gaussian	…X is not Gaussian
Linear function $Z = A \cdot X$	Z is Gaussian!	Z is **not** Gaussian
Non-linear function $Z = A(X)$	Z is **not** Gaussian	Z is **not** Gaussian

Gaussian + Linear transformation = again Gaussian!



See Example 3.7 in in **ProbObs2009**

Mean and Variance propagation laws

Looking at propagating first two moments

What we already know?

Let's consider a function $q: \mathbb{R}^m \to \mathbb{R}$ given m random variables:

$$X = q(\boldsymbol{Y}) = q(Y_1, Y_2, \dots, Y_m)$$

with known mean and covariance matrix for $\boldsymbol{Y}$ given by

$$\mathrm{E}\{\boldsymbol{Y}\} = \mu_Y, \qquad \mathrm{Var}\{\boldsymbol{Y}\} = \Sigma_Y$$

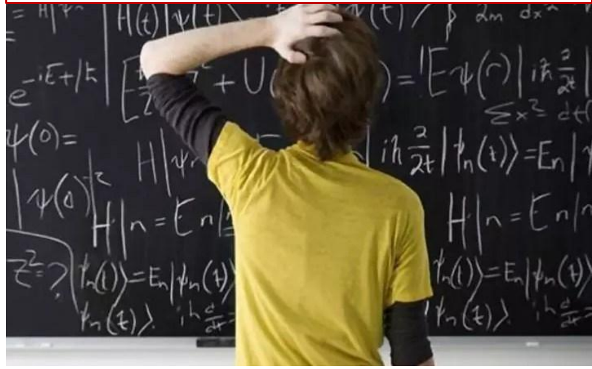
What we look for?

We would like to compute:

Mean	**Variance**
$\mathrm{E}\{\mathrm{X}\} = \mu_{\mathrm{X}},$	$\mathrm{Var}\{\mathrm{X}\} = \Sigma_{\mathrm{X}}$

Let's start simple… first *linear*, and then *non-linear* $q(\cdot)$

It is time for some board derivations



Linear function of one random variable

We consider $Y \in \mathbb{R}$ and $X \in \mathbb{R}$ given by

$$X = q(Y) = a \cdot Y + c$$

where

$$\mathrm{E}\{Y\} = \mu_Y, \qquad \mathrm{Var}\{Y\} = \sigma_Y^2$$

SOLUTION

We obtain

$$\mathrm{E}\{X\} = a \cdot \mathrm{E}\{Y\} + c = a \cdot \mu_Y + c$$

$$\mathrm{Var}\{X\} = a^2 \cdot \mathrm{Var}\{Y\} = a^2 \cdot \sigma_Y^2$$

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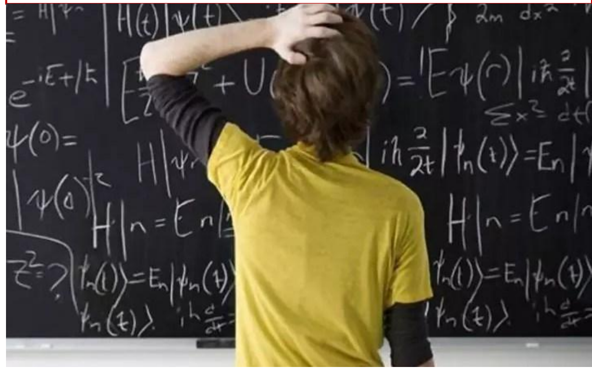


Linear function of two random variables

We consider $\boldsymbol{Y} \in \mathbb{R}^2$ and $X \in \mathbb{R}$ given by

$$X = q(\boldsymbol{Y}) = a_1 \cdot Y_1 + a_2 \cdot Y_2 + c$$

where

$$\mathrm{E}\{\boldsymbol{Y}\} = \boldsymbol{\mu}_{\boldsymbol{Y}} = \begin{pmatrix} \mu_1 \\ \mu_2 \end{pmatrix}, \qquad \mathrm{Var}\{Y\} = \Sigma_Y = \begin{bmatrix} \sigma_1^2 & \sigma_{12} \\ \sigma_{21} & \sigma_2^2 \end{bmatrix}$$

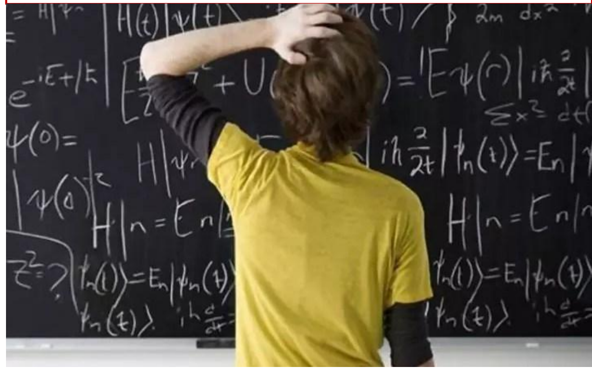
SOLUTION

We obtain

$$\mathrm{E}\{X\} = a_1 \cdot \mathrm{E}\{Y_1\} + a_2 \cdot \mathrm{E}\{Y_2\} + c = a_1 \cdot \mu_1 + a_2 \cdot \mu_2 + c$$

$$\mathrm{Var}\{X\} = (a_1, a_2) \cdot \mathrm{Var}\{Y\} \cdot \begin{pmatrix} a_1 \\ a_2 \end{pmatrix} = a_1^2\sigma_1^2 + a_2^2\sigma_2^2 + 2a_1a_2\sigma_{12}, \qquad \sigma_{12} = \mathrm{Cov}(Y_1, Y_2)$$

It is time for some board derivations



Linear function of n random variables

We consider $\boldsymbol{Y} \in \mathbb{R}^n$ and $X \in \mathbb{R}^m$ given by

$$X = q(\boldsymbol{Y}) = A\boldsymbol{Y} + \boldsymbol{c}$$

where

$$\mathrm{E}\{\boldsymbol{Y}\} = \boldsymbol{\mu_Y} \in \mathbb{R}^n, \qquad \mathrm{Var}\{Y\} = \Sigma_Y \in \mathbb{R}^{n\times n}$$

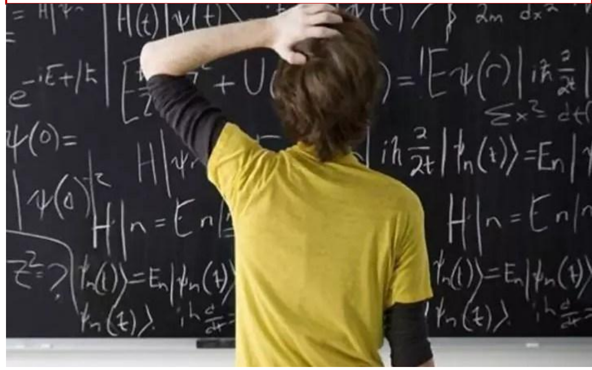
SOLUTION

We obtain

$$\mathrm{E}\{X\} = A\,\mathrm{E}\{\boldsymbol{Y}\} + \boldsymbol{c}$$

$$\mathrm{Var}\{X\} = A\Sigma_Y A^T$$

It is time for some board derivations



Non-Linear function of one random variable

We consider $Y \in \mathbb{R}$ and $X \in \mathbb{R}$ given by

$$X = q(Y) \approx q(\mu_Y) + \frac{dq}{dY}_{|\mu_Y}(Y - \mu_Y) + \frac{1}{2!}\frac{d^2q}{dY^2}_{|\mu_Y}(Y - \mu_Y)^2$$

where

$$\mathrm{E}\{Y\} = \mu_Y, \qquad \mathrm{Var}\{Y\} = \sigma_Y^2$$

SOLUTION

We obtain

$$\mathrm{E}\{X\} = \mathrm{E}\{q(Y)\} \approx q(\mu_Y) + \overset{=0}{\cancel{\frac{dq}{dY}_{|\mu_Y}(Y - \mu_Y)}} + \boxed{\frac{1}{2}\frac{d^2q}{dY^2}_{|\mu_Y}\sigma_Y^2}$$ Mean-bias term

$$\mathrm{Var}\{X\} = \mathrm{Var}\{q(Y)\} \approx \left(\frac{dq}{dY}_{|\mu_Y}\right)^2 \sigma_Y^2 + h.o.t.$$

It is time for some board derivations

Non-Linear function of n random variables

SOLUTION

We obtain… a terrific expression ☺

$$\mathrm{E}\{X\} = \mathrm{E}\{q(Y)\} \approx q(\mu_Y) + \frac{1}{2}\sum_{i}^{n} \frac{\partial^2 q}{\partial Y_i^2}\bigg|_{\mu_Y} \sigma_i^2 + \frac{1}{2}\sum_{i=1}^{n}\sum_{\substack{j=1 \\ j\neq 1}}^{n} \frac{\partial^2 q}{\partial Y_i \partial Y_j}\bigg|_{\mu_Y} Cov\left(Y_i, Y_j\right)$$

$$\mathrm{Var}\{X\} = \mathrm{Var}\{q(Y)\} \approx \sum_{i}^{n} \left(\frac{\partial q}{\partial Y_i}\bigg|_{\mu_Y}\right)^2 \sigma_i^2 + \sum_{i=1}^{n}\sum_{\substack{j=1 \\ j\neq 1}}^{n} \left(\frac{\partial q}{\partial Y_i}\bigg|_{\mu_Y}\right)\left(\frac{\partial q}{\partial Y_j}\bigg|_{\mu_Y}\right) Cov\left(Y_i, Y_j\right)$$

Let's describe each element step by step…

Monte Carlo simulations for uncertainty propagation

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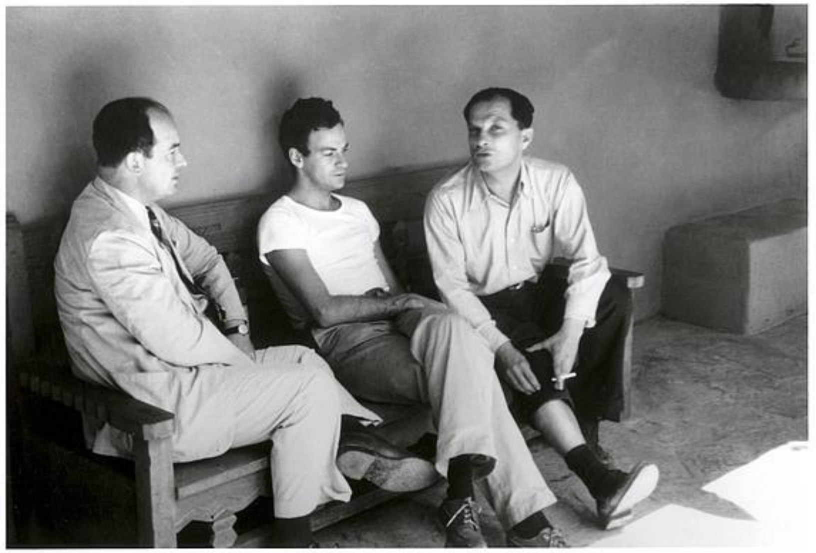
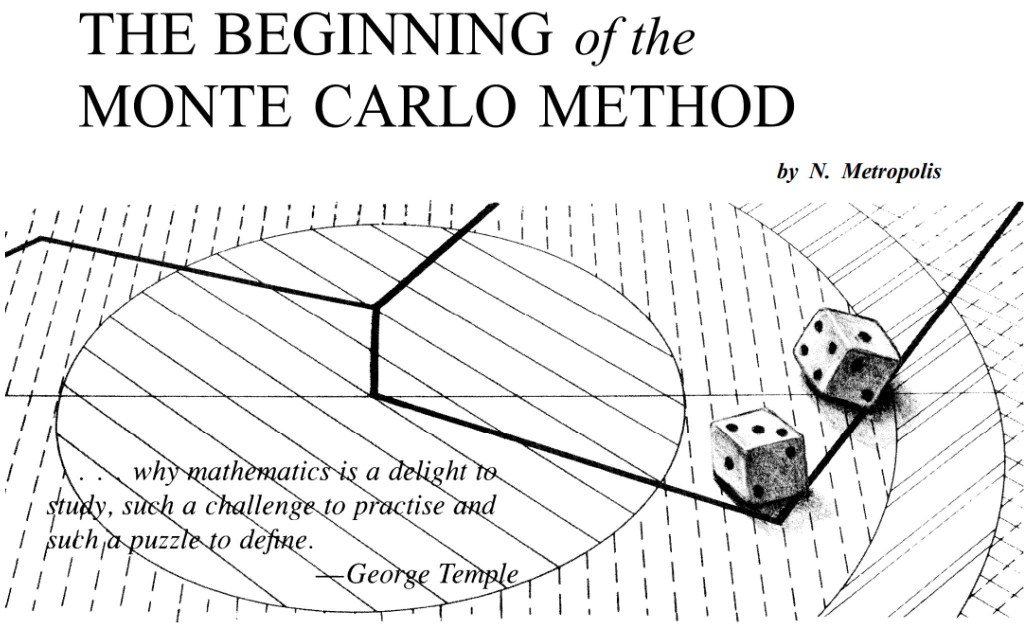
Monte Carlo methods

Historical background

It originated in 1946 by **Stanislaw Ulam**, and later in collaboration with **John von Neumann** to solve deterministic problems using a probabilistic procedure.



Left to Right: John von Neumann, Richard Feynman, and Stanislaw Ulam, at Bandelier National Monument near Los Alamos, 1949.



Metropolis, N. (1987). The beginning of the Monte Carlo method. *Los Alamos Science*, *15*, 125-130.

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Simulating Mean & Variance of transformed variables

General principle

From the Expectation and Variance laws, we consider

$$\mathrm{E}\{\mathrm{X}\} = \mathrm{E}\{q(Y)\} \approx \frac{1}{N}\sum_{i}^{N} q(Y_i) \equiv \hat{\mu}_X$$

$$\mathrm{Var}\{\mathrm{X}\} = \mathrm{Var}\{q(Y)\} \approx \frac{1}{N-1}\sum_{i}^{N} [q(Y_i) - \hat{\mu}_X][q(Y_i) - \hat{\mu}_X]^T$$

therefore, it represents a numerical approximation.

QUESTION: why using $N-1$ for the variance?

Simulating Mean & Variance of transformed variables

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QUESTION: why using $N-1$ for the variance?
Because we are making use of sample mean $\hat{\mu}_X$,
and so Var{X} becomes an *unbiased* estimator.

Simulating Mean & Variance of transformed variables

General principle

From the Expectation and Variance laws, we consider

$$\mathrm{E}\{\mathrm{X}\} = \mathrm{E}\{q(Y)\} \approx \frac{1}{N}\sum_{i}^{N} q(Y_i) \equiv \hat{\mu}_X \longrightarrow \text{np.mean(x)}$$

$$\mathrm{Var}\{\mathrm{X}\} = \mathrm{Var}\{q(Y)\} \approx \frac{1}{N-1}\sum_{i}^{N} [q(Y_i) - \hat{\mu}_X][q(Y_i) - \hat{\mu}_X]^T \longrightarrow \text{np.var(x, ddof=1)}$$

therefore, it represents a numerical approximation.

QUESTION: why using $N-1$ for the variance?
Because we are making use of sample mean $\hat{\mu}_X$,
and so Var{X} becomes an *unbiased* estimator.

Numerical exercise

Comparing Taylor and MC simulations

For the **Taylor (1st order) expansion**, we will proceed as discussed before.

For the **Monte Carlo simulations**, instead we will

1. Generate N samples from $Y \sim \mathcal{N}(\mu_Y, \Sigma_Y)$, e.g. assumed to be normally distributed;
2. Propagate each sample Y_i using the non-linear transformation, i.e. $X_i = q(Y_i)$;
3. Compute the (<u>unbiased</u>) sample mean and variance from $X_i, \forall i = 1 \ldots N$.

Barometric formula for an adiabatic atmosphere

Given an ideal gas with constant lapse rate, the Barometric law is

$$p(h) = p_0 \left(1 - \frac{L}{T_0} h\right)^{\kappa}, \qquad \kappa = \frac{g}{R_d L} \approx 5.256$$

which defines a non-linear dependence of atmospheric pressure on altitude.

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Relevant quantities:

- p_0 is the standard atmospheric pressure at sea level, e.g. $101{,}325\ \mathrm{Pa}$;
- L is the temperature lapse rate, e.g. $0.0065\ \frac{\mathrm{K}^{\circ}}{\mathrm{m}}$;
- h is the height (in meters) above mean sea level;
- T_0 is the sea-level reference temperature (in Kelvin), e.g. $288.15\ \mathrm{K}^{\circ}$;
- g is the gravitational acceleration near Earth's surface, e.g. $9.80665\, m/s^2$;
- R_d is the specific gas constant for dry air, e.g. $287.05\ \mathrm{J}\left(\mathrm{kg}/\mathrm{K}^{\circ}\right)^{-1}$;

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Example with univariate distribution: $h \sim \mathcal{N}\left(\mu_h, \sigma_h^2\right)$

Taylor (1st order) approximation

We have

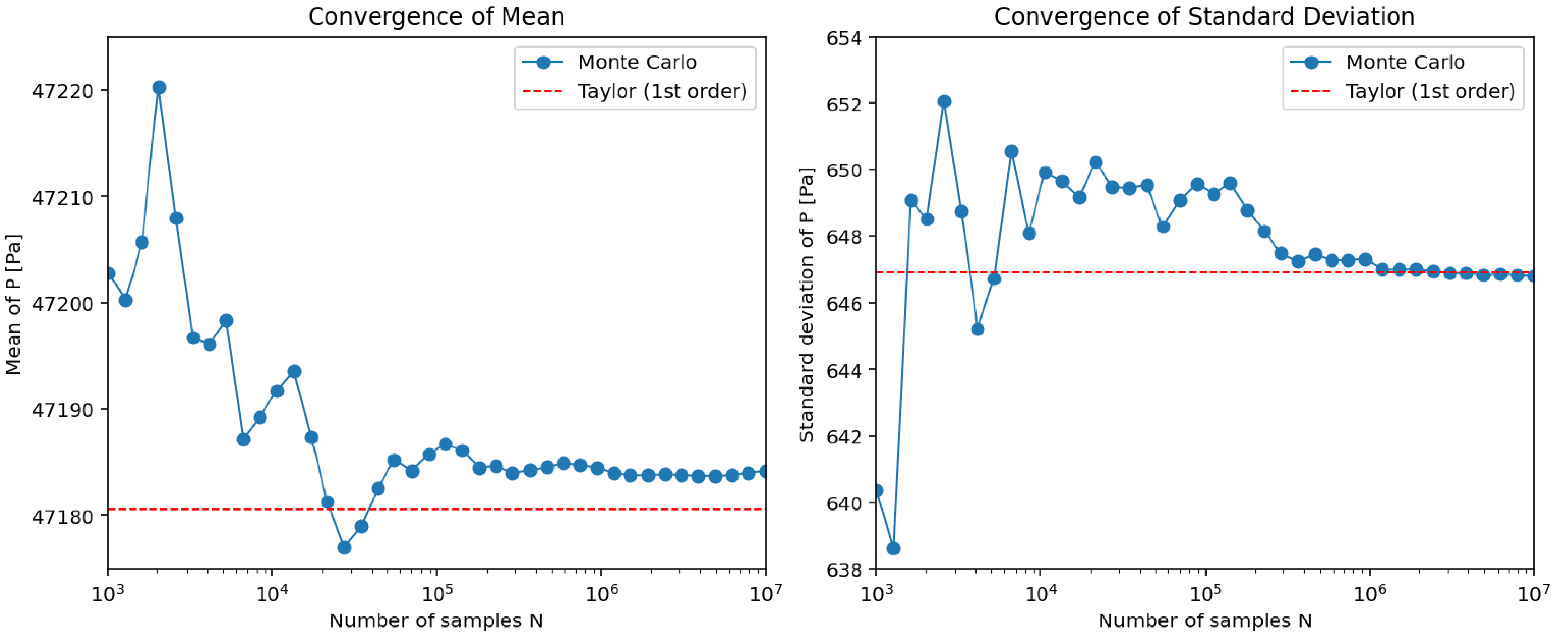
where

$$\frac{dp(\mu_h)}{dh} = -\frac{\alpha \cdot \kappa}{1 - \alpha \cdot \mu_h} p(\mu_h), \qquad \alpha = \frac{L}{T_0}$$

Monte Carlo simulations

Generate samples up to $N = 10^7$, then compute Mean & Standard Deviation (i.e. $\sqrt{Var}$)

Comparison results for different number of samples



Example with univariate distribution: $h \sim \mathcal{N}\left(\mu_h, \sigma_h^2\right)$

Taylor (2nd order) approximation

We have

$$E\big(p(h)\big) \approx p(\mu_h) + \frac{\sigma_h^2}{2}\frac{d^2p(\mu_h)}{dh^2}, \qquad Var\big(p(h)\big) \approx \sigma_h^2 \cdot \left(\frac{dp(\mu_h)}{dh}\right)^2$$

where

$$\frac{d^2p(\mu_h)}{dh^2} = -\frac{\alpha^2 \cdot \kappa(\kappa-1)}{(1-\alpha\cdot\mu_h)^2}p(\mu_h), \qquad \alpha = \frac{L}{T_0}$$

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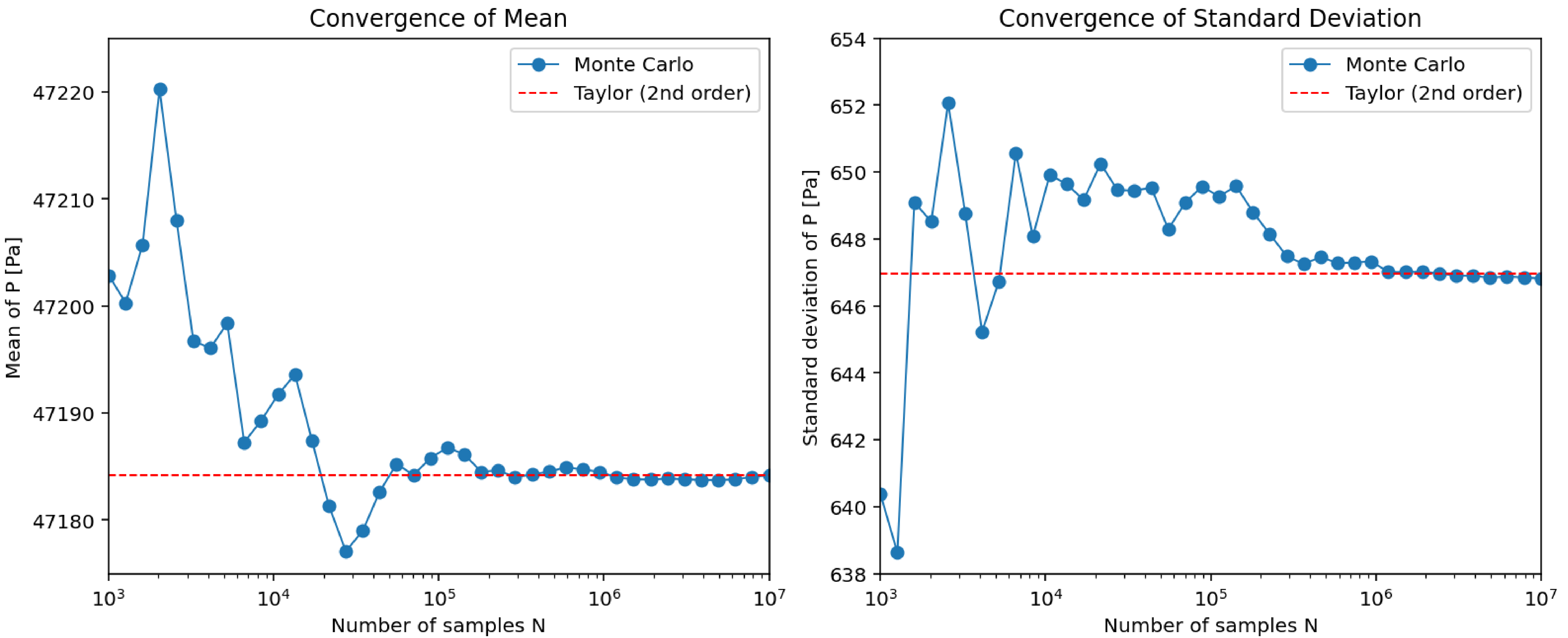
Generate samples up to $N = 10^7$, then compute Mean & Standard Deviation (i.e. $\sqrt{Var}$)

Comparison results for different number of samples



Time for last few questions…

What happens if we

- Increase or decrease the **expected value** μ_h?

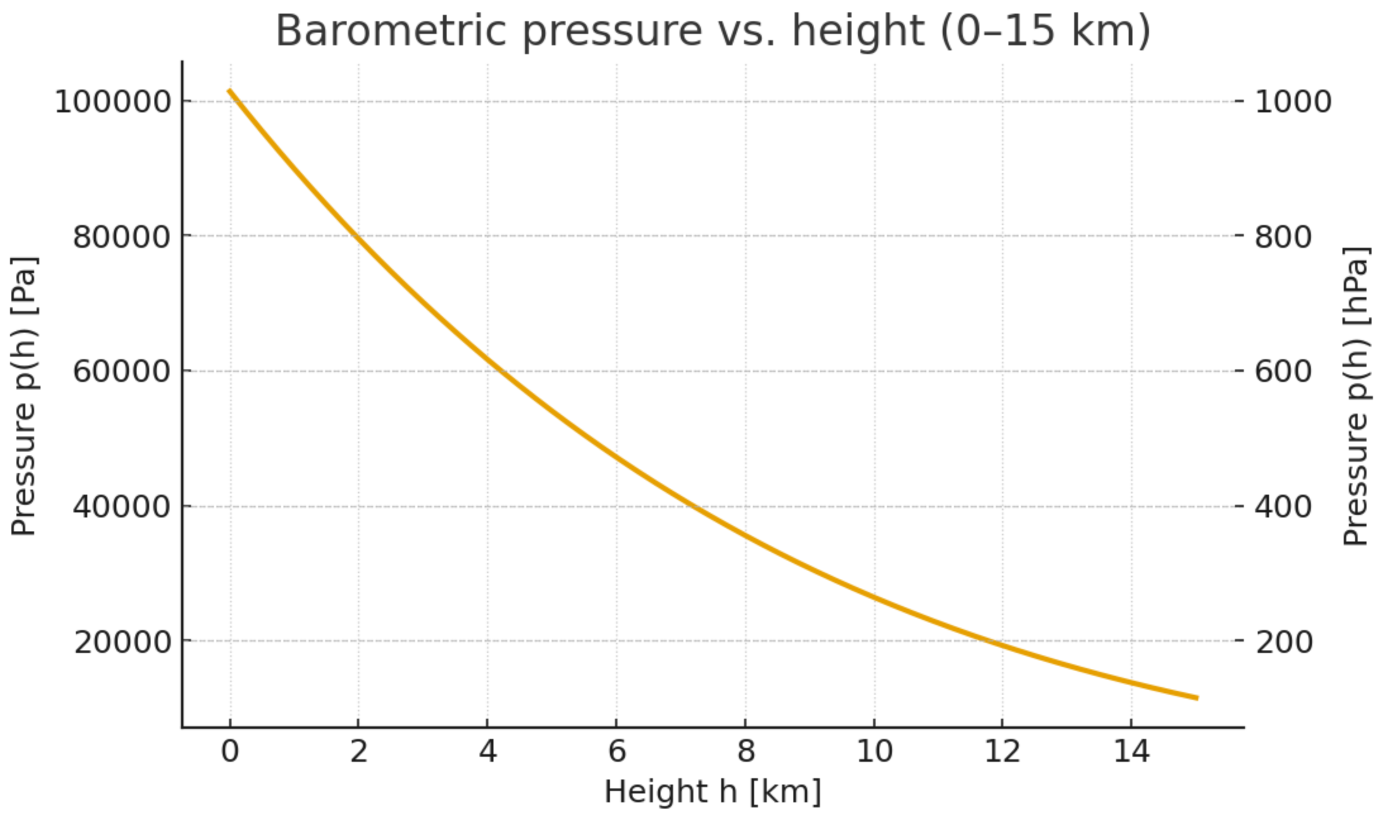
Time for last few questions…

<u>What happens if we</u>

- Increase or decrease the **expected value** μ_h?

  Then $E\big(p(h)\big)$ surely changes, but errors in the approximation are quite similar…

  e.g. see derivatives.



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Time for last few questions…

<u>What happens if we</u>

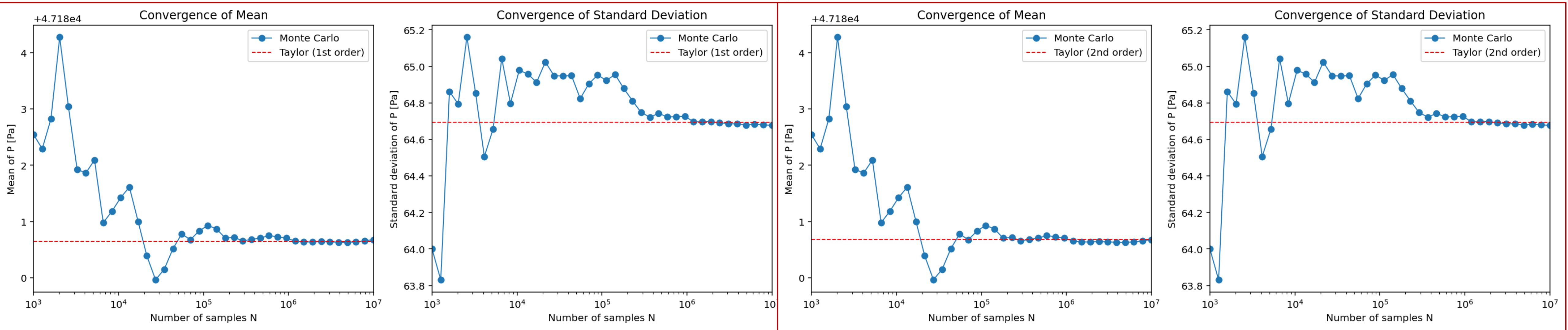
- Increase or decrease the **standard deviation** σ_h?

Time for last few questions…

What happens if we

- Increase or decrease the **standard deviation** σ_h?
  - If larger, then $\sigma_{p(h)}$ approximation gets poorer, but…
  - if smaller, then $\sigma_{p(h)}$ approximation is better! ☺

Results for $\sigma_h = 10\ [m] \ll \sigma_h^{\mathrm{OLD}}$



Summary

Conclusions

Lessons (hopefully) learned

In this class, we have seen

- How a **transformation of random variables** affects their distribution;
- How first moments of the distribution can be propagated for **linear** transformations;
- How first moments of the distribution can be propagated for **non-linear** transformations;
- How **Monte Carlo simulations** can be adopted for propagating the uncertainty.

Conclusions

Remember, if…	…X is Gaussian	…X is not Gaussian
Linear function $Z = A \cdot X$	Z is Gaussian!	Z is **not** Gaussian
Non-linear function $Z = A(X)$	Z is **not** Gaussian	Z is **not** Gaussian

Lessons (hopefully) learned

In this class, we have seen

- How a **transformation of random variables** affects their distribution;
- How first moments of the distribution can be propagated for **linear** transformations;
- How first moments of the distribution can be propagated for **non-linear** transformations;
- How **Monte Carlo simulations** can be adopted for propagating the uncertainty.

Lastly, remember… only Gaussian distribution + Linear transformation = **Gaussian again!**

What's next?

- Key information from today's lecture can be found in the **textbook**, i.e. https://mude.citg.tudelft.nl/book/2025/propagation_uncertainty/overview.html

- **Wednesday's workshop:**

  i.e. have fun with uncertainty propagation of Mean and Variance.

- **Friday's project:**

  i.e. group assignment (graded!), again on propagation & MC simulations.

And enjoy the journey!

NOTICE : your “journey” is often a non-linear function! ☺