Introduction to Uncertainty Quantification
Module 3.2: Expansion Methods for Uncertainty Propagation

1 Taylor Series Expansions

For simple functions and certain systems that are either close to linear or have small uncertainties, a common approach is to expand the function in terms of a Taylor series expansion. Using this expansion, we show that it is straightforward to express the lower-order moments (i.e. mean and variance) of the output in terms of the moments of the input through simple analytical expressions. For this reason, the methods described below employing Taylor series expansions are often referred to as *propagation of moments* or *moment propagation methods.*

1.1 Functions of Random Variables

Consider a function $Y = f(X)$, where X is a random variable having mean value $\mu_X = \mathbb{E}[X]$ and variance $V_X = \mathrm{Var}(X) = \mathbb{E}[(X - \mu_X)^2]$. If the function is infinitely differentiable at μ_X, we can express the function through the *Taylor Series Expansion* about μ_X as follows:

$$Y(X) = \sum_{n=0}^{\infty} \frac{1}{n!} \frac{d^n f(\mu_X)}{dX^n} (X - \mu_X)^n \tag{1}$$

It is common to truncate this sum to include just a small number of terms. The *first-order* Taylor series expansion includes truncates for $n = 1$ and includes only *linear* terms as follows:

$$Y(X) \approx f(\mu_X) + (X - \mu_X) \frac{df(\mu_X)}{dX}. \tag{2}$$

Likewise, the *second-order* Taylor series expansion truncates for $n = 1$ and includes only *linear* and *quadratic* terms as follows:

$$Y(X) \approx f(\mu_X) + (X - \mu_X) \frac{df(\mu_X)}{dX} + \frac{1}{2}(X - \mu_X)^2 \frac{d^2 f(\mu_X)}{dX^2}. \tag{3}$$

Recognizing that Y is a random variable, we can easily compute its moments by applying our moment operations to these expressions. For example, the first-order approximate mean value can be computed as follows:

$$\begin{aligned} \mu_Y = \mathbb{E}[Y] &\approx \mathbb{E}[f(\mu_X)] + E\left[(X - \mu_X)\frac{df(\mu_X)}{dX}\right] \\ &\approx f(\mu_X) \end{aligned} \tag{4}$$

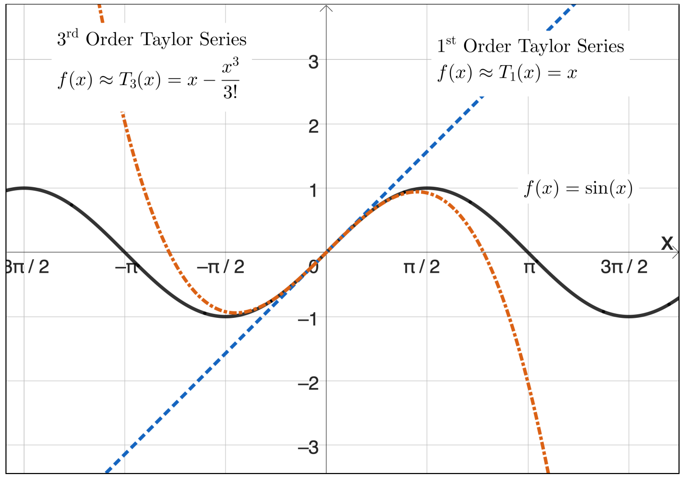

Figure 1: Taylor series approximations for $f(x) = \sin(x)$.

where we recognize that $\mathbb{E}[f(a)] = f(a)$ and $\mathbb{E}[X - \mu_X] = \mathbb{E}[X] - \mu_X = 0$. Likewise, we can express the first-order variance as:

$$
\begin{aligned}
V_Y = \text{Var}(Y) &\approx \mathbb{E}\left[(Y - \mu_Y)^2\right] \\
&\approx \mathbb{E}\left[\left(f(\mu_X) + (X - \mu_X)\frac{df(\mu_X)}{dX} - f(\mu_X)\right)^2\right] \\
&\approx \mathbb{E}\left[\left((X - \mu_X)\frac{df(\mu_X)}{dX}\right)^2\right] \\
&\approx \text{Var(X)}\left(\frac{df(\mu_X)}{dX}\right)^2
\end{aligned}
\tag{5}
$$

Here we see that we can derive the first and second-order moments of the output Y simply as a function of the moments of the inputs X. Determining the mean value of Y requires knowing only the mean value of X, while determining the variance of Y requires knowing only the variance of X. We can similarly derive second-order approximations of the mean μ_Y and variance V_Y using the Taylor series approximation in Eq. (3). This will be conducted as an exercise.

1.2 Functions of Random Vectors

Consider a function $Y = f(\boldsymbol{X})$, where $\boldsymbol{X} = [X_1, X_2, \ldots, X_n]^T$ is a random vector having mean vector $\boldsymbol{\mu_X} = [\mathbb{E}[X_1], \mathbb{E}[X_2], \ldots, \mathbb{E}[X_n]]^T$ and covariance matrix $\boldsymbol{C_X}$. If the function is infinitely differentiable at $\boldsymbol{\mu_X}$, we can express the function through the *Taylor Series Expansion* about $\boldsymbol{\mu_X}$ in a similar manner as the univariate case. Due to the complexity of the expression, we won't provide it here. We will focus only on the first and second-order expansions.

The *first-order* Taylor series expansion of multiple variables can be expressed as:

$$
Y \approx f(\boldsymbol{\mu_X}) + \sum_{i=1}^{n} [X_i - \mu_{X_i}] \frac{\partial f(\boldsymbol{\mu_X})}{\partial X_i} \tag{6}
$$

and the *second-order* Taylor series expansion is given by:

$$Y \approx f(\boldsymbol{\mu_X}) + \sum_{i=1}^{n}[X_i - \mu_{X_i}]\frac{\partial f(\boldsymbol{\mu_X})}{\partial X_i} + \frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n}[X_i - \mu_{X_i}][X_j - \mu_{X_j}]\frac{\partial^2 f(\boldsymbol{\mu_X})}{\partial X_i \partial X_j} \tag{7}$$

Again, applying expectation to the approximation of Y, we can estimate its moments as follows. The mean can be computed as:

$$\begin{aligned} \mu_Y = \mathbb{E}[Y] &\approx \mathbb{E}[f(\boldsymbol{\mu_X})] + \mathbb{E}\left[\sum_{i=1}^{n}(X_i - \mu_{X_i})\frac{\partial f(\boldsymbol{\mu_X})}{\partial X_i}\right] \\ &\approx \mathbb{E}[f(\boldsymbol{\mu_X})] = \mathbb{E}[f(\mathbb{E}[X_1], \mathbb{E}[X_2], \ldots, \mathbb{E}[X_n])] \end{aligned} \tag{8}$$

where we recognize that each term in the summation $\mathbb{E}[X_i - \mu_{X_i}] = 0$.

The first-order variance can be expressed as

$$\begin{aligned} V_Y = \mathrm{Var}(Y) &\approx \mathbb{E}\left[(Y - \mu_Y)^2\right] \\ &\approx \mathbb{E}\left[f(\boldsymbol{\mu_X}) + \sum_{i=1}^{n}[X_i - \mu_{X_i}]\frac{\partial f(\boldsymbol{\mu_X})}{\partial X_i} + \frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n}[X_i - \mu_{X_i}][X_j - \mu_{X_j}]\frac{\partial^2 f(\boldsymbol{\mu_X})}{\partial X_i \partial X_j}\right] \\ &\approx \sum_{i=1}^{n}\sum_{j=1}^{n}\frac{\partial f(\boldsymbol{\mu_X})}{\partial X_i}\frac{\partial f(\boldsymbol{\mu_X})}{\partial X_j}\mathrm{Cov}(X_i, X_j) \end{aligned} \tag{9}$$

We once again see that we can determine the moments of Y from the moments of $\boldsymbol{X}$. Estimating the mean of Y requires knowing the mean vector of $\boldsymbol{X}$, $\boldsymbol{\mu_X}$. Estimating the variance of Y requires knowing the complete covariance matrix of $\boldsymbol{X}$, $\boldsymbol{C_X}$.

1.3 Example

The bending stress, F, in a beam can be expressed through the following simple expression:

$$F = \frac{My}{I} \tag{10}$$

where M is the applied bending moment, y is the distance from the neutral axis, and I is the moment of inertia of the beam. Consider that M and I are independent random variables with means μ_M and μ_I and variances σ_M^2 and σ_I^2. Approximate the first-order mean and variance of the bending stress.

First-Order Mean Bending Stress

$$\mu_F \approx f(\mu_M, \mu_I) = \frac{\mu_M y}{\mu_I} \tag{11}$$

First-Order Variance of Bending Stress

$$\begin{aligned} \sigma_F^2 &\approx \left(\frac{\partial F(\mu_M, \mu_I)}{\partial M}\right)^2 \sigma_M^2 + \left(\frac{\partial F(\mu_M, \mu_I)}{\partial I}\right)^2 \sigma_I^2 + 2\left(\frac{\partial F(\mu_M, \mu_I)}{\partial M}\right)\left(\frac{\partial F(\mu_M, \mu_I)}{\partial I}\right)\mathrm{Cov}(M, I) \\ &\approx \left(\frac{y}{\mu_I}\right)^2 \sigma_M^2 + \left(\frac{\mu_M y}{\mu_I^2}\right)^2 \sigma_I^2 \end{aligned} \tag{12}$$

where we notice that, because M and I are independent, we have $\mathrm{Cov}(M, I) = 0$.

2 Perturbation Methods

Consider that the n-dimensional input random vector $\boldsymbol{X}$ has probability density function $p_{\boldsymbol{X}}(\boldsymbol{X})$ that is symmetric in each component X_i around a nominal value $\bar{x}$. The random vector $\boldsymbol{X}$ can be expressed in terms of its nominal components and some perturbations δX as:

$$\boldsymbol{X} = \bar{\boldsymbol{x}} + \delta\boldsymbol{X} = [\bar{x}_1 + \delta X_1, \bar{x}_2 + \delta X_2, \ldots, \bar{x}_n + \delta X_n] \tag{13}$$

The vector of perturbations $\delta\boldsymbol{X}$ about $\bar{\boldsymbol{x}}$ are typically assumed to be equal to one standard deviation and may, for example, correspond to error bars in a measurement. However, in general the perturbations $\delta\boldsymbol{X}$ may be any well-defined deviation or error that is symmetric around $\bar{\boldsymbol{x}}$ such that $\boldsymbol{X}$ admits the representation in Eq. (13).

Consider now a function $Y = f(\boldsymbol{X}) = f(\bar{x}_1 + \delta x_1, \bar{x}_2 + \delta x_2, \ldots, \bar{x}_n + \delta x_n)$. We can again apply the 2^{nd}-order Taylor series expansion to obtain:

$$\begin{aligned} Y = f(\boldsymbol{X}) &= f(\bar{x}_1 + \delta x_1, \bar{x}_2 + \delta x_2, \ldots, \bar{x}_n + \delta x_n) \\ &\approx f(\bar{\boldsymbol{x}}) + \sum_{i=1}^{n} \frac{\partial f(\bar{\boldsymbol{x}})}{\partial X_i}\delta X_i + \frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n} \frac{\partial^2 f(\bar{\boldsymbol{x}})}{\partial X_i \partial X_j}\delta X_i \delta X_j \end{aligned} \tag{14}$$

Let us denote the partial derivatives by $s_i = \dfrac{\partial f(\bar{\boldsymbol{x}})}{\partial X_i}$, which we refer to as the *sensitivity* of $f(\boldsymbol{X})$ to parameter X_i evaluated at $\bar{\boldsymbol{x}}$. These sensitivities may also be referred to as *local sensitivities* since they correspond to the derivative evaluated locally at $\bar{\boldsymbol{x}}$. Using these sensitivities, we can express the *first-order* (linear) Taylor series expansion as

$$f(\boldsymbol{X}) \approx f(\bar{\boldsymbol{x}}) + \sum_{i=1}^{n} s_i \delta X_i \tag{15}$$

The first and second-order moments of the random vector $\boldsymbol{X}$ can be expressed as:

$$\begin{aligned} \mathbb{E}[X_i] &= \bar{x}_i \\ V_{X_i} = \mathrm{Var}(X_i) &= \int_{\mathbb{R}^n} (x_i - \bar{x}_i)^2 p_{\boldsymbol{X}}(\boldsymbol{x}) d\boldsymbol{x} = \int_{\mathbb{R}^n} (\delta X_i)^2 d\boldsymbol{x} \\ \mathrm{Cov}(X_i, X_j) &= \int_{\mathbb{R}^n} (x_i - \bar{x}_i)(x_j - \bar{x}_j) p_{\boldsymbol{X}}(\boldsymbol{x}) d\boldsymbol{x} = \int_{\mathbb{R}^n} \delta X_i \delta X_j p_{\boldsymbol{X}}(\boldsymbol{x}) d\boldsymbol{x} \end{aligned} \tag{16}$$

Using these expressions and the first-order Taylor series expansion, the mean value $\mathbb{E}[Y] = \mathbb{E}[f(\boldsymbol{X})]$ is given by

$$\begin{aligned} \mathbb{E}[Y] = \mathbb{E}[f(\boldsymbol{X})] &\approx f(\bar{\boldsymbol{x}}) \int_{\mathbb{R}^n} p_{\boldsymbol{X}}(\boldsymbol{x}) d\boldsymbol{x} + \sum_{i=1}^{n} s_i \int_{\mathbb{R}^n} (x_i - \bar{x}_i) p_{\boldsymbol{X}}(\boldsymbol{x}) d\boldsymbol{x} \\ &\approx f(\bar{\boldsymbol{x}}) \end{aligned} \tag{17}$$

where the first integral is equal to one and the second integral is equal to zero. The variance of $Y = f(\boldsymbol{X})$

can be given by

$$\begin{aligned}\mathrm{Var}(f(\boldsymbol{X})) &= \mathbb{E}[(f(\boldsymbol{X}) - f(\bar{\boldsymbol{x}}))^2] \\ &\approx \int_{\mathbb{R}^n} \left(\sum_{i=1}^{n} s_i \delta X_i\right) \left(\sum_{j=1}^{n} s_j \delta X_j\right) p_{\boldsymbol{X}}(\boldsymbol{x}) d\boldsymbol{x} \\ &\approx \sum_{i=1}^{n}\sum_{j=1}^{n} s_i s_j \int_{\mathbb{R}^n} \delta X_i \delta X_j p_{\boldsymbol{X}}(\boldsymbol{x}) d\boldsymbol{x} \\ &\approx \sum_{i=1}^{n}\sum_{j=1}^{n} s_i s_j \mathrm{Cov}(X_i, X_j)\end{aligned} \tag{18}$$

Collecting the sensitivities in a vector $\boldsymbol{s} = [s_1, s_2, \ldots, s_n]^T$ we can express the variance V_Y using the following matrix relation:

$$V_Y = \boldsymbol{s}^T \boldsymbol{C_X} \boldsymbol{s} \tag{19}$$

where $\boldsymbol{C_X}$ is the covariance matrix of $\boldsymbol{X}$ having terms given in Eq. (16).

2.1 Special Case: Normal Random Variables

The first order Taylor series approximates the function by a linear expression. As a result, if $\boldsymbol{X}$ is a normal random vector having mean vector $\boldsymbol{\mu_X}$ and covariance matrix $\boldsymbol{C_X}$, then the first order Taylor series approximation of $Y = f(\boldsymbol{X})$ is also normal having distribution:

$$Y = f(\boldsymbol{X}) \sim N(f(\boldsymbol{\mu_X}), S\boldsymbol{C_X}S^T) \tag{20}$$

Nomenclature

Functions

$P(\cdot)$ Probability measure

$f_X(x)$ Probability density function (PDF) of a random variable X

$f_{\boldsymbol{X}}(\cdot)$ Joint probability density function of the random vector $\boldsymbol{X}$

$F_X(x)$ Cumulative distribution function (CDF) of a random variable X

$F_{\boldsymbol{X}}(\cdot)$ Joint Cumulative Distribution Function of the random vector $\boldsymbol{X}$

Operators

$\cap$ Intersection

Variables

X A random variable

$\boldsymbol{X}$ A random vector in $\mathbb{R}^n$

μ_X Mean of the random variable X

σ_X Standard deviation of the random variable X

$\boldsymbol{J}$ Jacobian matrix of a function