Stochastic Collocation

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1 Introduction

The concept behind using stochastic collocation for propagating uncertainty is that the uncertainty space can be spanned by quadrature rules deterministically instead of using stochastic sampling.

2 Uncertainty

TODO -realizations

2.1 Uncertain Variables

We consider a given variable x with some uncertainty in value. We define \bar{x} as the average value of this variable. The uncertainty in x can be given in several ways. In this work we consider two types of uncertainty: uniform and normal.

2.1.1 Uniformly-Uncertain Variables

A uniformly-uncertain variable, hereafter referred to as uniform variable, has an equal probability of being realized at all its potential values. For example, for a six-sided die, each face is equally probable to end facing up when the die is rolled. For a continuous uniform variable, the range of realizations are well-described by an average value \bar{x} , minimum value $\bar{x} - \sigma$, and maximum value $\bar{x} + \sigma$. We note the following characteristics of uniform variables:

- The possible values of x range linearly from $\bar{x} \sigma$ to $\bar{x} + \sigma$.
- The possible values of x as a function of w are found along $x(w) = \sigma w + \bar{x}$.
- The probability of any realization w is given by a horizontal distribution P(w) which has a value of 1/2 from -1 to 1 and is zero everywhere else.

2.2 Uncertain Processes

TODO

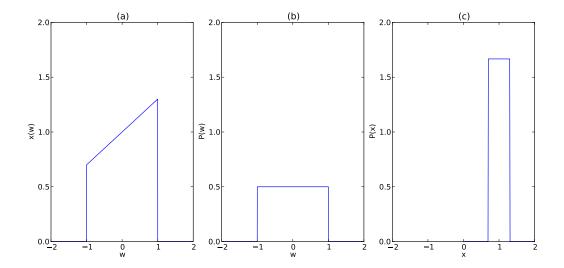


Figure 1: (a) Possible values of x(w) as a function of w. (b) Probability distribution of w. (c) Probability distribution of x(w).

3 Quadrature

Gaussian quadrature makes the following assumption:

$$\int_{a}^{b} f(x)dx = \int_{a}^{b} g(x)P(x)dx \approx \sum_{n=1}^{N} w_{n}f(x_{n}), \tag{1}$$

where f(x) is any function continuous over the interval $a \to b$, P(x) is a probability distribution function for x, N is the order of quadrature chosen and w_n and x_n are given by the choice of quadrature and its order. In general x_n are referred to as the abscissas of the quadrature, and w_n as the associated weights. In the limit that N approaches infinity, the quadrature is exact.

There are many different Gaussian quadrature sets that may are selected based on their abscissa distribution and the limits a and b of the integral in question.

3.1 Implementing Integration with Quadrature

Here we pause to make a note of the methods surrounding evaluating integrals using quadrature sets. We consider in particular an implemented function integrate(f(x)) that accepts a function and integrates it using quadrature. In general, as above, a quadrature evaluates an integral using some weighting function P(x), not to be confused with the quadrature weights w_n . The Legendre quadrature is singular because its weighting function is 1; this means that f(x) = g(x) for Legendre quadrature, and a function integrateLegendre(f(x)) that uses Legendre quadrature will integrate f(x) exactly as expected.

For other quadrature sets, however, $P(x) \neq 1$ and a function such as integrateHermite(f(x)) will not accurately return $\int f(x)dx$. Use of these quadrature sets require some knowledge of the user, since the integration routine will actually integrate $\int f(x)P(x)dx$. In the case of Hermite quadrature, $P(x) = \exp(-x^2)$, so integrateHermite(f(x)) would return $\int f(x) \exp(-x^2)dx$. This

is useful for a user that wants to integrate a function times a weighting factor by only passing the function.

3.2 Gauss-Legendre

Gauss-Legendre quadrature spans [-1,1] with P(x) = 1, and is perhaps the most commonly used quadrature in particle transport. The abscissa are given by finding the roots of the Legendre polynomials

$$P_N(x) = \frac{1}{2^N N!} \frac{d^N}{dx^N} [(x^2 - 1)^N], \tag{2}$$

and the weights are given by

$$w_n = \frac{2}{(1 - x_n^2)[P_N'(x_n)]^2}. (3)$$

Gauss-Legendre quadrature is well-suited for spanning the uncertainty space of uniformly-distributed uncertainty.

3.3 Gauss-Hermite

Gauss-Hermite quadrature spans $[-\infty, \infty]$ and $W(x) = e^{-x^2}$. The abscissa come from the roots of the physicist's Hermite polynomial

$$H_N(x) = (-1)^N e^{x^2} \frac{d^N}{dx^N} e^{-x^2},$$
(4)

and the weights are given by

$$w_n = \frac{2^{N-1}N!\sqrt{\pi}}{N^2[H_{N-1}(x_n)]^2}. (5)$$

Gauss-Hermite quadrature is well-suited for spanning the uncertainty space of normally-distributed uncertainty; however, careful consideration must be made of the probability function associated with choosing the Hermite quadrature. Since we are most interested in using Hermite quadrature to span the uncertainty space of a variable with normal (Gaussian)-distributed uncertainty, we desire the probability distribution to be normal; that is, we desire the probability distribution to be $P(x) = e^{-x^2/2}$, noting the half in the numerator. We can adjust our integral to agree well with the normal distribution probability function by defining

$$b \equiv \frac{a}{\sqrt{2}}, \qquad a = \sqrt{2}b. \tag{6}$$

The integral we desire to approximate using the normal distribution is

$$\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(a)e^{a^2/2} da \approx \sum_{i} w_i f(a_i). \tag{7}$$

Replacing $b\sqrt{2}$ for a everywhere restores the Hermite form of the integral,

$$\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(b\sqrt{2})e^{b^2} \sqrt{2}db \approx \sum_{i} \frac{w_i}{\sqrt{\pi}} f(b_i \sqrt{2}). \tag{8}$$