Polynomial Chaos Expansions for Uncertainty Quantification

AICES EU Regional School 2016 - Part 1

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Users of simulations always push the limits

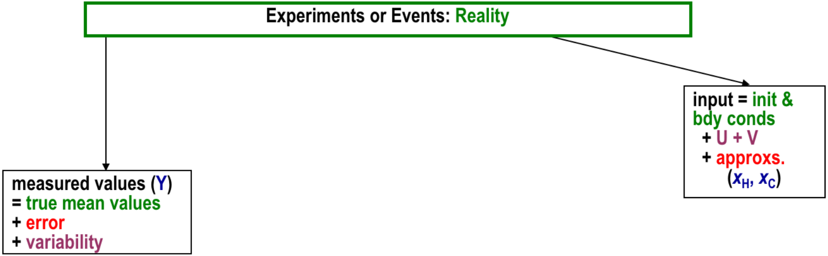
- No matter the hardware, software, or problem at hand when a user wants to solve a problem using simulation,
- The user will usually pick the resolution, tolerances, etc. based on how long it will take to get the answer.
- This means that no matter how advanced the numerical techniques we develop, the users will want more.
- When we ask the question, what are the uncertainties in a calculation?
- The answer usually requires many simulation runs (when all we could afford originally is one simulation).
- As a result, we necessarily want to minimize the number of simulation runs that are required to measure the uncertainty in a simulation.

What do I mean by Uncertainty

Experiments or Events: Reality

1

What do I mean by Uncertainty



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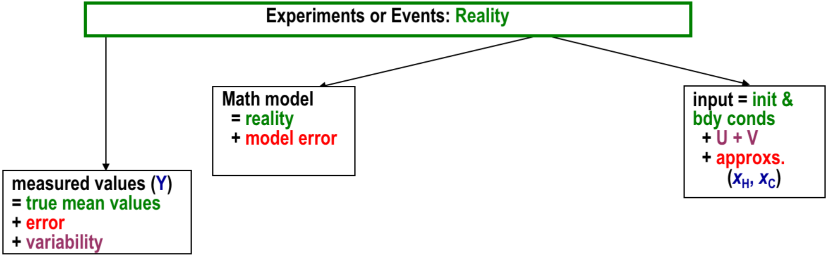

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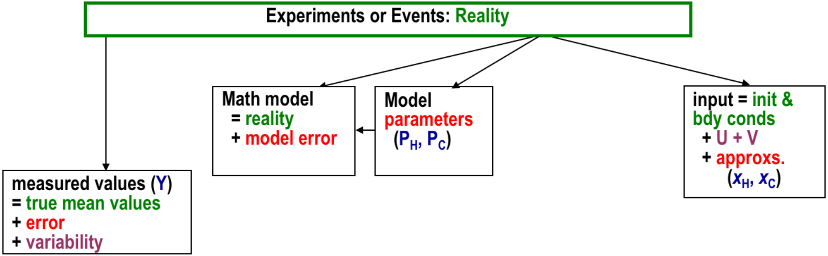

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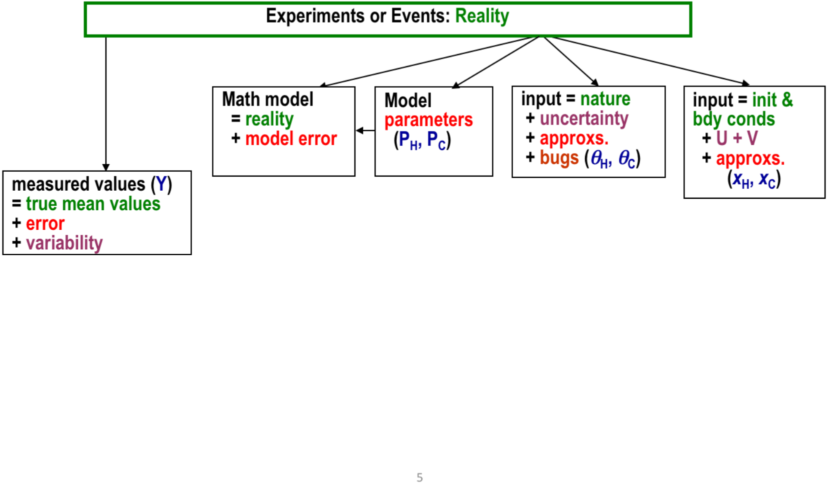

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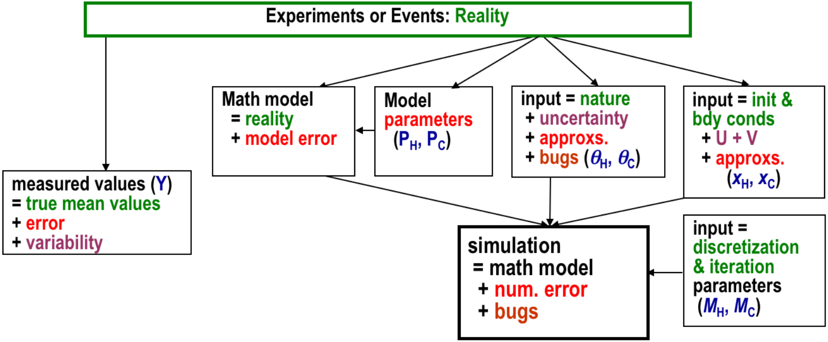

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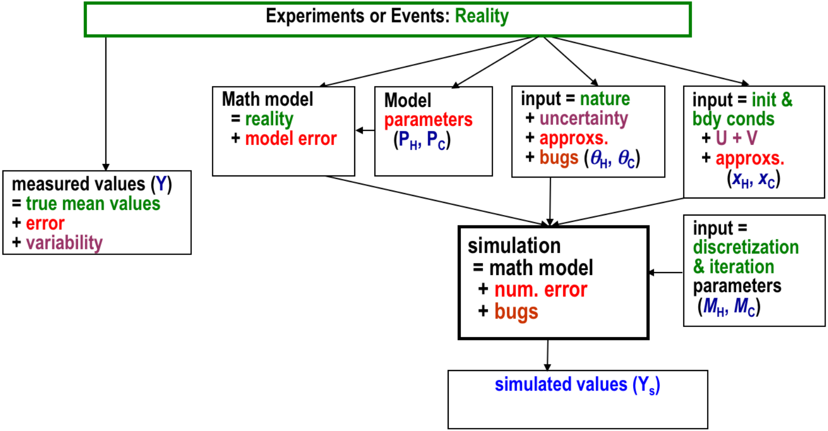

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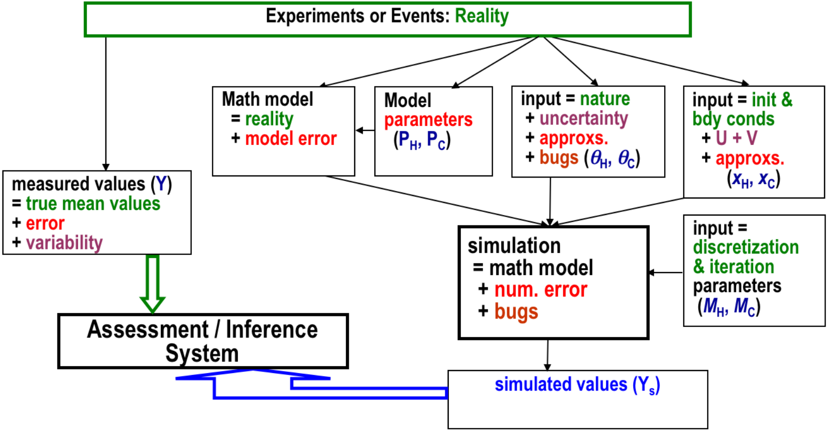

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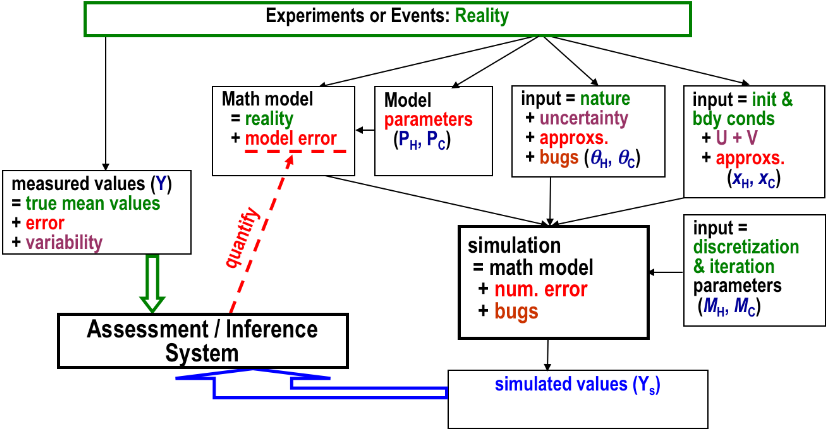

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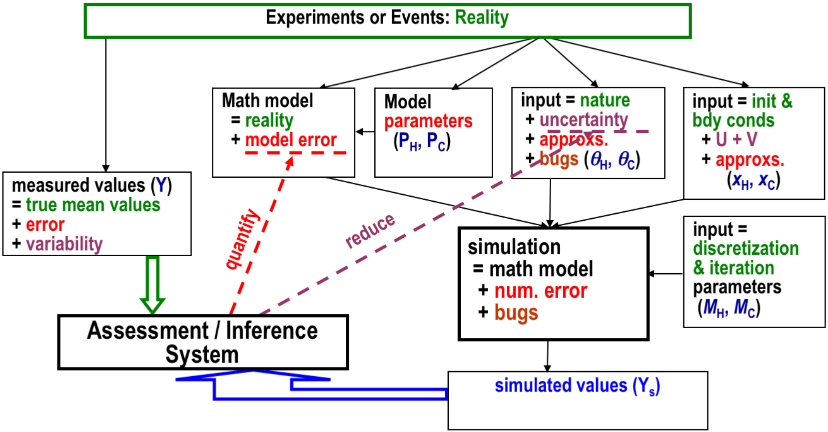

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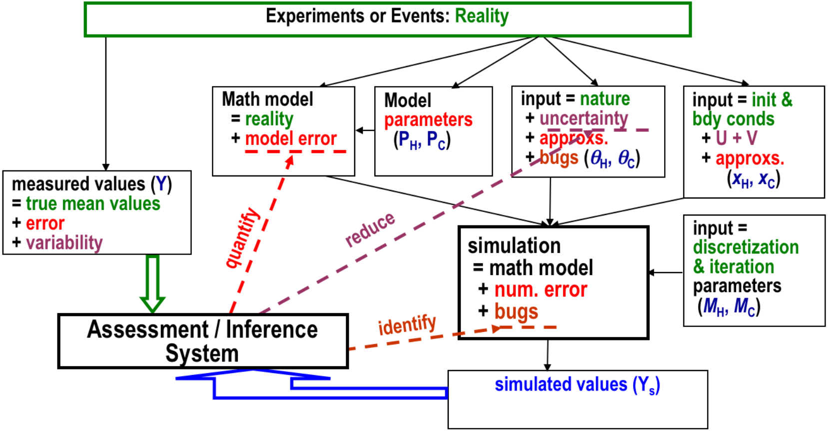

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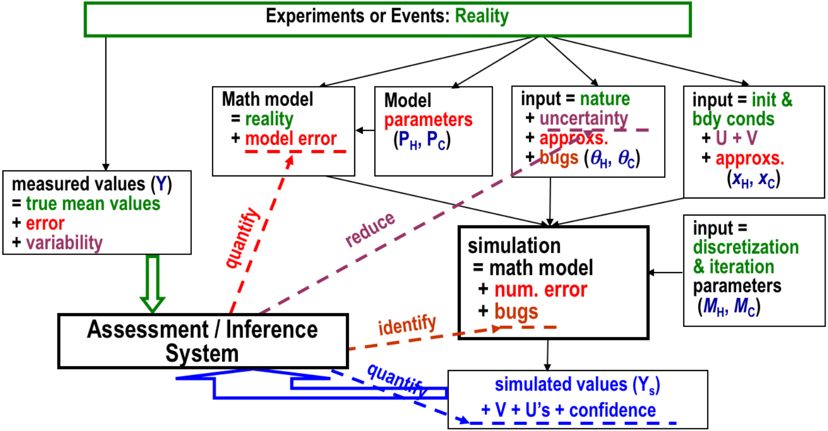

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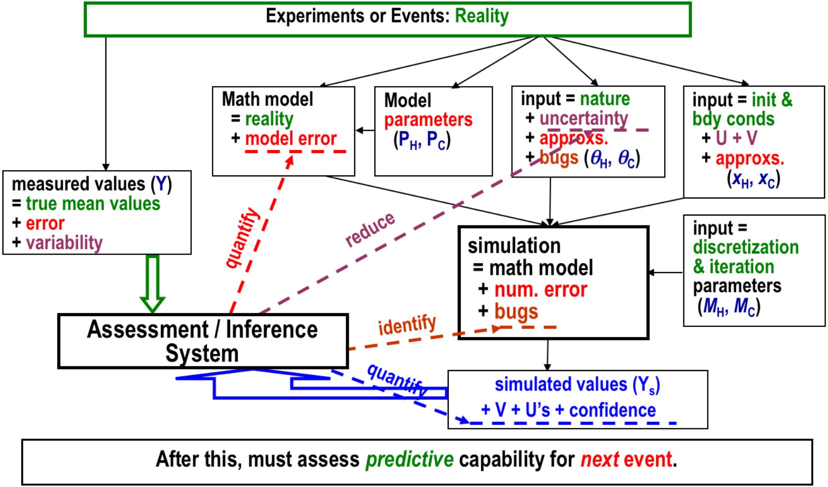

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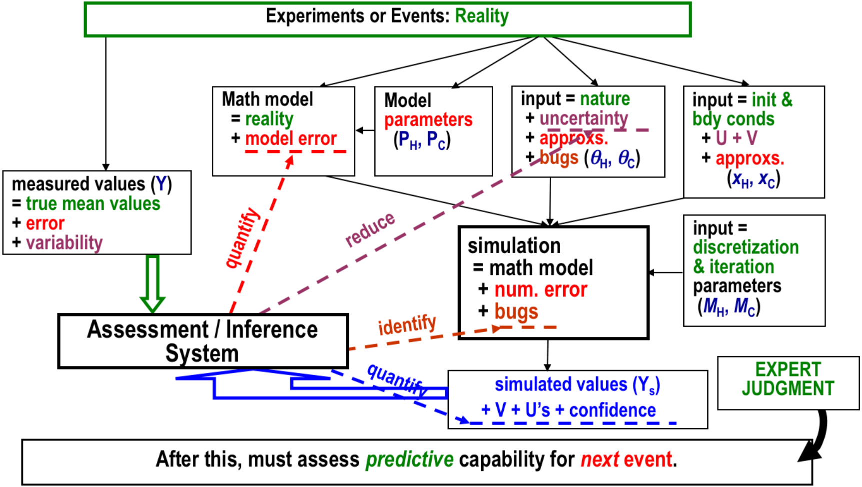


For this talk we need to reduce the scope

A few brief words on the parts of the process we will not dive into

- Quantifying model error is very difficult need either a higher-fidelity model to compare to or more experiments
  - Of course all of the other uncertainties can influence the comparison.
- Reducing the uncertainty of constants of nature involves models for those constants often, are we trying to get the right value or calibrate?
- Identifying bugs in a simulation code requires extensive comparison with known solutions, checking convergence rates, nightly regression tests, software quality assurance, etc., etc.
- Can never really get rid of expert judgment when we want to extend simulation to something we don't have experimental data for.

Parametric Uncertainty Quantification

In this discussion, we will focus how uncertainties in inputs to the simulation affect the output.

- The inputs parameters can be properties of the system (geometry or material properties) as well as boundary and initial conditions., as well as ambient conditions.
- These can be influenced by manufacturing tolerances, lack of knowledge of material properties, inherent uncertainty in ambient conditions.
- Consider the simple model for the distance traveled by a projectile launched with velocity, v, angle θ:

$$\mathrm{d} = \frac{\mathrm{v}^2 \sin(2\theta)}{\mathrm{g}}.$$

- Here the uncertain parameters are v, θ, and g.

More Assumptions on the Inputs

Some of the usual messiness of real life will be ignored here:

- We assume that the distributions of the input parameters are known.
- For example, we could say that a parameter is normally distributed with a known mean and variance.
- Coming up with these distributions almost always requires assumptions about the tails of the distribution.
- We also assume that the parameters are independent.
- It is possible to generalize to non-independent parameters or to transform dependent parameters to independent parameters.

Quantities of Interest

In uncertainty quantification (UQ) we want to start with the end in mind.

- What are the truly important outputs of the simulation. Typically these are integrals over the solution to the underlying mathematical model. We call these integral quantities quantities of interest (QoI).
    - Given uncertainty in the inputs to climate models, what is the predicted temperature rise ($\mathrm{QoI} = \Delta T$)?
    - How much of the heat shield on a space vehicle will be ablated during re-entry ($\mathrm{QoI} = m_{\mathrm{loss}}$)?
- While we are interested in the solution everywhere in space/time/etc., success or failure of the system is determined by the QoI.
- In many analyses, adding more QoI's does not make the analysis more time consuming.
- If you are interested in the solution everywhere, you can turn the solution into a finite number of QoI using the Karhunen-Loeve transform.

Calculating QoI

Consider a mathematical model that describes our system

$$L(x,t;\Theta)u(x,t;\Theta) = q(x,t;\Theta),$$

where x and t are deterministic parameters, and Θ contains the uncertain parameters with known distributions. The solution to this system u gives us the quantity of interest

$$\mathrm{QoI} = \mathrm{QoI}[u(x,t;\Theta)].$$

Basic Monte Carlo Procedure

Given distributions for the random variables Θ, we can perform the following iteration procedure.

1. Sample the input parameters from their respective distributions.
2. Run a simulation with the sampled input parameters.
3. Calculate the QoI from the outputs.
4. Repeat N times

This procedure will generate N samples from the output distribution, but will requires N simulations to be run. If each simulation takes hours or days to run, then you want to make N as small as possible.

Basic Monte Carlo Procedure

Monte Carlo has several properties

- It is extremely robust: given enough samples it will give the correct answer.
- Because we are getting samples of the distribution for each QoI, we can compute any function of those distributions that we would like.
- Monte Carlo is insensitive to the number of input parameters,
- The downside is that estimates derived from Monte Carlo, e.g., the mean of the distribution, have an expected error that decays as $\mathrm{N}^{-1/2}$.
- That is, to cut the expected uncertainty in a quantity estimated via Monte Carlo, we need to quadruple the number of samples.
- There are approaches to improve Monte Carlo (e.g., quasi-Monte Carlo or stratified sampling) but these often give up other nice properties of the method.

Section 3

Expanding the distribution in terms of orthogonal polynomials

- An alternative approach is to write the QoI as an expansion in orthogonal polynomials.
- In particular we will pick the orthogonal polynomials so that the weighting function in the orthogonality condition "matches" the distribution of the parameters.
- To compute the integrals in the expansion we will use a collocation procedure and Gauss quadrature.
- In the process we will encounter many classic approximation techniques and have to review a host of statistics, special functions, and quadrature techniques.

Expanding the distribution in terms of orthogonal polynomials

- These expansions are called polynomial chaos expansions.
- If the quantity of interest is a smooth function of the random variables, then we expect the expansion to be accurate with only a few terms.
- The benefit of spectral projection is, like Monte Carlo, it is an non-intrusive method:
  - Existing codes and methods can be applied out of the box.
- The approach does suffer from the curse of dimensionality in that the number of terms in the expansion explodes as the dimension of the random variable space increases.
- We will discuss approaches to mitigate this, using sparse grids and compressed sensing techniques.

Matching Input Distributions to Orthogonal Polynomials

Input Distribution	Orthogonal Polynomial	Support
Normal	Hermite	$(-\infty, \infty)$
Uniform	Legendre	$[a, b]$
Beta	Jacobi	$[a, b]$
Gamma	Laguerre	$[0, \infty)$

1: The orthogonal polynomials and support corresponding to the different families of input random variables.

Notation

- Throughout this work we will use capital italic letters to denote a random variable, e.g., X, and lower case italics to denote a realization or single value of that random variable x.
- Additionally, the tilde will be used to indicate how a random variable is distributed, and
- Calligraphic letters to denote a specific type of distribution.
- For example, shortly we will write $X \sim \mathcal{N}(\mu, \sigma^2)$ to indicate that the random variable X is a normal (or Gaussian) random variable with mean μ and variance σ^2.

Probability Density Function

- We consider a continuous random variable, X, that is distributed as a normal, also called Gaussian, random variable.
- A real, continuous random variable is defined by its probability density function, $f(x)$, which is defined so that

$$f(x)dx = \text{The probability that the random variable } X \text{ takes a value in } dx \text{ about } x.$$

By this definition the following normalization is natural,

$$\int_{-\infty}^{\infty} f(x)\, dx = 1,$$

because it implies that the random variable takes on a value somewhere on the real line.

Probability Density Function

The probability density function (PDF) for a normal random variable is given by

$$f(x \mid \mu, \sigma^2) = \frac{1}{\sqrt{2\sigma^2\pi}} e^{-\frac{(x-\mu)^2}{2\sigma^2}}, \tag{1}$$

where the parameters of the distribution are

- μ, the mean of the distribution,
- σ, the standard deviation of the distribution and its square, σ^2, which is called the variance.

This PDF integrates to one, as can easily be checked.

Cumulative Distribution Function

Related to the probability distribution is the cumulative density function (CDF), $F(x)$, which is defined as

$$F(x) = \text{The probability that the random variable } X \text{ takes a value less than or equal to } x. \tag{2}$$

There are two relationships between the CDF and the PDF from basic calculus

$$F(x) = \int_{-\infty}^{x} f(x')\,dx', \qquad f(x) = \frac{dF}{dx}. \tag{3}$$

The CDF is a non-decreasing and right continuous function. It also has the property that the difference in two values of the CDF is the probability that the random variable is in a range:

$$F(b) - F(a) = \int_{a}^{b} f(x)\,dx = P(a < X \leq b).$$

Cumulative Distribution Function

- The CDF for a normal random variable can be written in terms of the error function

$$F(x \mid \mu, \sigma^2) = \frac{1}{2}\left[1 + \operatorname{erf}\left(\frac{x-\mu}{\sigma\sqrt{2}}\right)\right]. \tag{4}$$

- A normal random variable, with a given μ and σ^2 is often written as

$$X \sim \mathcal{N}(\mu, \sigma^2).$$

Expectation Value

- The expectation value of a function of a random variable is the integral of the function times the PDF. In particular, for a function $g(x)$ the expectation is written as

$$E[g(X)] = \int_{-\infty}^{\infty} g(x)f(x)\,dx. \tag{5}$$

- The mean of a random variable is the expectation of the variable itself. The mean is sometimes written as $\bar{x}$:

$$\bar{x} = E[X] = \int_{-\infty}^{\infty} xf(x)\,dx. \tag{6}$$

Expectation Value

- The variance, is the difference of the expectation of x^2 and the square of the mean,

$$\mathrm{Var}(X) = \mathrm{E}[X^2] - \mathrm{E}[X]^2 = \int_{-\infty}^{\infty} x^2 f(x)\,dx - \left(\int_{-\infty}^{\infty} x f(x)\,dx\right)^2. \quad (7)$$

- For the normal distribution, we can see that μ is the mean by computing the integral

$$\bar{x} = \int_{-\infty}^{\infty} \frac{x}{\sqrt{2\sigma^2\pi}} e^{-\frac{(x-\mu)^2}{2\sigma^2}}\,dx = \mu.$$

- It can be shown than for a normal variable, $\mathrm{Var}(X) = \sigma^2$.

Standard Normal Random Variable

- There is a special case of the normal distribution, called the standard normal.
- This is a normal distribution with zero mean, and unit variance, i.e., $Z \sim \mathcal{N}(0,1)$.
- In this case, we give the PDF a special symbol, $\phi(z)$:

$$\phi(z) \equiv f(z \mid \mu = 0, \sigma^2 = 1) = \int_{-\infty}^{\infty} \frac{1}{\sqrt{2\pi}} e^{-\frac{z^2}{2}}. \tag{8}$$

- The CDF for the standard normal is written as $\Phi(x)$ and is defined as

$$\Phi(z) = F(z \mid \mu = 0, \sigma^2 = 1) = \frac{1}{2}\left[1 + \operatorname{erf}\left(\frac{z}{\sqrt{2}}\right)\right]. \tag{9}$$

Standard Normal Random Variable

- The standard normal is important because we can transform any normal random variable, $X \sim \mathcal{N}(\mu, \sigma^2)$, into a standard normal, $Z \sim \mathcal{N}(0, 1)$, via the transform:

$$z = \frac{x - \mu}{\sigma}. \tag{10}$$

- This relation shows that z is a measure of how many standard deviations from the mean a given value is.
- The inverse of this transform is

$$x = \mu + \sigma z. \tag{11}$$

Hermite Polynomials

- The Hermite polynomials, $\mathrm{He}_n(x)$, are a set of orthogonal polynomials that form a basis for square-integrable functions on the real line with weight,
$$w(x) = e^{-x^2/2},$$
and inner product
$$\langle g(x), h(x) \rangle = \int_{-\infty}^{\infty} g(x)h(x)\, e^{-\frac{x^2}{2}}\, dx,$$
i.e., the polynomials form an orthogonal basis for $L^2(\mathbb{R}, w(x)\,dx)$.
- Achtung: We use the "probabilist" version of the functions because of similarities with the standard normal distribution in the weighting function. There is also a "physicist" version defined to work well with the harmonic oscillator.
- The Hermite polynomials are defined as
$$\mathrm{He}_n(x) = (-1)^n e^{\frac{x^2}{2}} \frac{d^n}{dx^n} e^{-\frac{x^2}{2}}. \qquad (12)$$

Hermite Polynomials

The first few Hermite polynomials are

$$\begin{aligned} \mathrm{He}_0(x) &= 1, \\ \mathrm{He}_1(x) &= x, \\ \mathrm{He}_2(x) &= x^2 - 1, \\ \mathrm{He}_3(x) &= x^3 - 3x, \\ \mathrm{He}_4(x) &= x^4 - 6x^2 + 3, \\ \mathrm{He}_5(x) &= x^5 - 10x^3 + 15x. \end{aligned}$$

The orthogonality relation for the Hermite polynomials is

$$\int_{-\infty}^{\infty} \mathrm{He}_m(x)\mathrm{He}_n(x)\, e^{-\frac{x^2}{2}}\, dx = \sqrt{2\pi}\, n!\, \delta_{nm}. \tag{13}$$

Hermite Polynomials

The expansion of a function in terms of Hermite polynomials is written as

$$g(x) = \sum_{n=0}^{\infty} c_n \mathrm{He}_n(x), \tag{14}$$

where the expansion constants are given by

$$c_n = \frac{\langle g(x), \mathrm{He}_n(x) \rangle}{\sqrt{2\pi} n!}. \tag{15}$$

Hermite Expansion of Standard Normal

- Consider a function $g(X)$ where $X \sim \mathcal{N}(0,1)$.
- The value of the function is also a random variable that we will call $G \sim g(X)$.
- The value of c_0 is the mean of G

$$c_0 = \int_{-\infty}^{\infty} \frac{g(x)}{\sqrt{2\pi}} e^{-\frac{x^2}{2}} dx = E[G] = \bar{g}. \tag{16}$$

- Recall that the variance of G is given by $E[G^2] - E[G]^2$, which is equal to

$$\begin{aligned} \mathrm{Var}(G) &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \left(\sum_{n=0}^{\infty} c_n He_n(x) \right)^2 e^{-\frac{x^2}{2}} dx - c_0^2 \\ &= \frac{1}{\sqrt{2\pi}} \sum_{n=0}^{\infty} c_n^2 \langle He_n(x), He_n(x) \rangle - c_0^2 \\ &= \sum_{n=1}^{\infty} n! c_n^2. \end{aligned} \tag{17}$$

Example: $g(X) = \cos(x)$

- Let us consider the function $g(X) = \cos(x)$. In this case we can directly compute the expansion coefficients:

$$c_n = \frac{1}{\sqrt{2\pi} n!} \int_{-\infty}^{\infty} \cos(x) He_n(x) e^{-x^2/2} dx = \begin{cases} 0 & n \text{ odd} \\ (-1)^{\frac{n}{2}} \frac{e^{-1/2}}{n!} & n \text{ even} \end{cases}. \tag{18}$$

This makes the approximation to the function

$$\cos(X) = e^{-\frac{1}{2}} \sum_{n \text{ even}} (-1)^{\frac{n}{2}} \frac{He_n(x)}{n!}, \qquad X \sim \mathcal{N}(0,1). \tag{19}$$

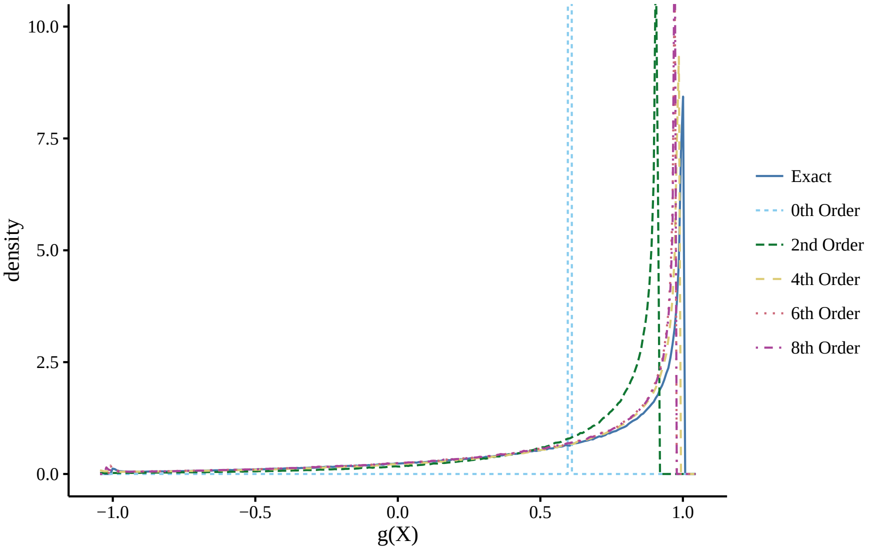
This implies that the mean of $g(x)$ is $e^{-1/2}$ and that the variance is

$$\mathrm{Var}(G) = e^{-1} \sum_{n \text{ even}, n>1} \frac{1}{n!} = e^{-1}(\cosh(1) - 1) \approx 0.19978820.$$

Example: $g(X) = \cos(x)$

- We can get a baseline for comparison between the expansion and the actual distribution of G.
- We do this by sampling a value for X from a standard normal and then evaluating $g(x)$ to get a Monte Carlo approximation to the true distribution of G.
  - In this case, each sample is a simulation.
- We then can compare that to the values obtained by sampling X and then evaluating the expansion in Eq. (19) with different orders of expansion.
  - In this case each sample involves just evaluating a polynomial (i.e., it is free).
- Of course this assumes we know the expansion.

Example: $g(X) = \cos(x)$, Different Expansion Orders



Example: $g(X) = \cos(x)$

- In these results we see that improvement obtained as we go to higher order expansions.
- The zeroth-order expansion only gives a value of the mean, and there is a large improvement in going to the second-order expansion.
- There is a noticeable difference between the fourth- and second-order expansions, though beyond that, there is little difference on in the figure
- We can track improvement in the higher-order expansions by looking at the convergence of the variance.

Example: $g(X) = \cos(x)$, Convergence of Variance

order	variance
0	0
2	0.183939721
4	0.199268031
6	0.199778974
8	0.199788098
∞	0.199788200

2: The convergence of $\mathrm{Var}(G)$ for $g(X) = \cos(x)$, where $X \sim \mathcal{N}(0,1)$.

Hermite Expansion of a function of a general normal random variable

- If the random variable is normal, but not standard normal, then we need to change the procedure a bit.
- Let's say that $g(X)$ is a function of the random variable $X \sim \mathcal{N}(\mu, \sigma^2)$.
- In this case we will change variables to express the function as $g(Z)$ where Z and X are related by Eq. ((11)).
- Therefore, in this case

$$c_n = \frac{\langle g(\mu + \sigma z), He_n(z) \rangle}{\sqrt{2\pi} n!}. \tag{20}$$

- The bounds of the inner product's integration are not affected because they are infinite, this may not be the case when we have different random variables.

Example: $g(X) = \cos(x)$

- Going back to our example from before where $g(X) = \cos(x)$, we now say that $X \sim \mathcal{N}(\mu = 0.5, \sigma^2 = 4)$.
- Performing the integrals for the coefficients in Eq. (20) gives the following expansion, to fifth order,

$$\cos(X) \approx e^{-2}\left(1 - 2\mathrm{He}_2(z) + \frac{2}{3}\mathrm{He}_4(z)\right)\cos\left(\frac{1}{2}\right) + e^{-2}\left(2\mathrm{He}_1(z) + \frac{4}{3}\mathrm{He}_3(z) - \frac{4}{15}\mathrm{He}_5(z)\right)\sin\left(\frac{1}{2}\right) \quad (21)$$

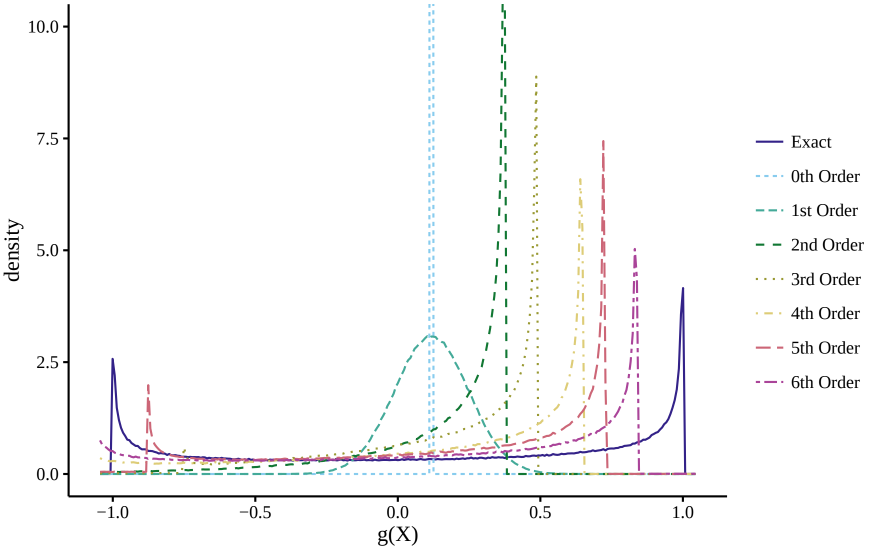
- The mean is

$$\bar{g} = e^{-2}\cos\left(\frac{1}{2}\right) \approx 0.1187678845769458,$$

- The variance is

$$\mathrm{Var}(G) = \frac{\left(e^4 - 1\right)\left(e^4 - \cos(1)\right)}{2e^8} \approx 0.4859848152088114144.$$

Example: $g(X) = \cos(x)$, Different Expansion Orders



Example: $g(X) = \cos(x)$, Convergence of Variance

order	variance
1	0.0168393
2	0.129686
3	0.174591
4	0.325053
5	0.360976
6	0.441223
7	0.454908
∞	0.485984815

3: The convergence of $\text{Var}(G)$ for $g(X) = \cos(x)$, where $X \sim \mathcal{N}(\mu = 0.5, \sigma^2 = 4)$.

Why Quadrature?

- Recall that our ultimate goal is to use polynomial expansions to provide information about the distribution of output quantities from a computer simulation.
- To that end we will need to estimate the coefficients in the Hermite expansion.
- If we use a quadrature rule to estimate the integrals in these coefficients, then we would like a quadrature rule to require as few evaluations of the integrand as possible,
  - Each evaluation requires running a new simulation at a different point in input space.

Gauss-Hermite Quadrature

The most common way to approximate the required integrals is to use Gauss-Hermite quadrature, which is a Gauss quadrature rule for computing integrals of the form

$$\int_{-\infty}^{\infty} f(x)e^{-x^2}\,dx \approx \sum_{i=1}^{n} w_i f(x_i), \tag{22}$$

where the abscissas, x_i, are given by the n roots of $He_n(x)$, and the weights are given by

$$w_i = \frac{\sqrt{\pi}n!}{n^2\left(He_{n-1}\left(\sqrt{2}x_i\right)\right)^2}. \tag{23}$$

The abscissas are symmetric about 0.

Gauss-Hermite Quadrature

n	$\lvert x_i \rvert$	w_i
1	0	$\sqrt{\pi}$
2	$\frac{1}{\sqrt{2}}$	$\frac{1}{2}\sqrt{\pi}$
3	0	$\frac{2}{3}\sqrt{\pi}$
	$\frac{1}{2}\sqrt{6}$	$\frac{1}{6}\sqrt{\pi}$
4	0.524647623275290	0.804914090005514
	1.65060123885785	0.0813552017779922
	0	0.945308720482942
5	0.958572464613819	0.393619323152240
	2.02018270456086	0.0199532688074820
	0.436077411927617	0.724629595224391
6	1.335849074013697	0.157067320322856
	2.350604973674492	0.00453000990550885

Gauss-Hermite Quadrature: Watch Out

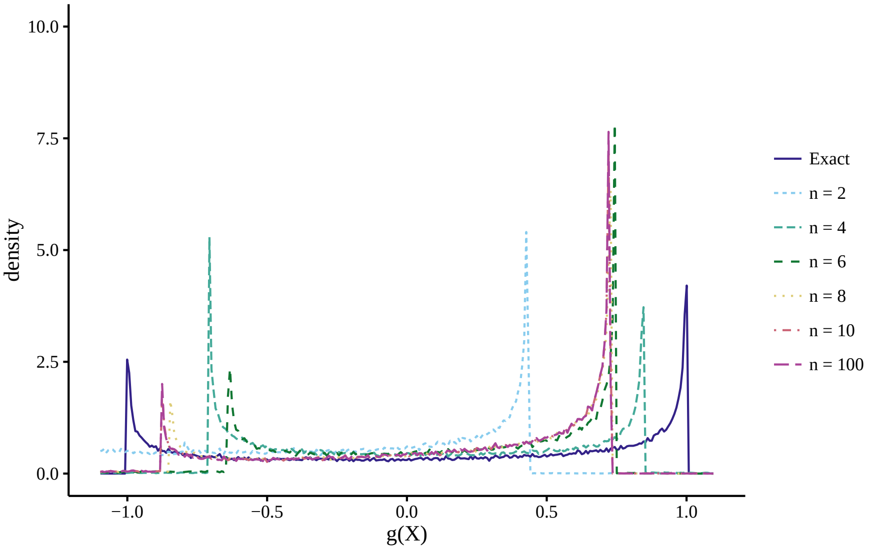
- There is a slight issue in Gauss-Hermite quadrature in that it uses the a weight function of $\exp(-x^2)$, rather than $\exp(-x^2/2)$ we used in our inner product definition.
- Therefore, we need to make the change of variable $x \to x'/\sqrt{2}$.
- This makes the approximation to the inner product

$$\langle g(x), He_m(x)\rangle \approx \sqrt{2}\sum_{i=1}^{n} w_i g(\sqrt{2}x_i) \tag{24}$$

Gauss-Hermite Quadrature: $g(X) = \cos x$ example

- We can use our previous example, of $g(X) = \cos(x)$, where $X \sim \mathcal{N}(\mu = 0.5, \sigma^2 = 4)$, as a test of estimating the inner-products using Gauss-Hermite quadrature rules.
- On the next slide, the distribution, as approximated by a fifth-order Hermite expansion, is computed using Gauss-Hermite quadratures of different values of n.
- We need at least 8 quadrature points to get an accurate estimate of the coefficients.
- Also, we look at the convergence of the coefficients as a function of the number of quadrature points.
- Here we see that to estimate the mean, c_0, with two-digits of accuracy we need $n = 6$, whereas the c_5 term needs $n = 9$ to get that many digits of accuracy.

Gauss-Hermite Quadrature: $g(X) = \cos x$ order 5



Gauss-Hermite Quadrature: $g(X) = \cos x$ coefficients

n	c_0	c_1	c_2	c_3	c_4	c_5
2	-0.365203	-0.435940	-0.000000	0.145313	0.030434	-0.021797
3	0.307609	0.087730	-0.569973	-0.000000	0.142493	-0.004386
4	0.065646	-0.219271	-0.023343	0.173281	0.000000	-0.034656
5	0.130446	-0.103803	-0.322800	0.037629	0.141446	0.000000
6	0.116662	-0.135589	-0.213171	0.104748	0.048382	-0.028531
7	0.119090	-0.128702	-0.242956	0.081489	0.089843	-0.012370
8	0.118725	-0.129931	-0.236549	0.087602	0.076377	-0.018886
9	0.118773	-0.129744	-0.237688	0.086315	0.079768	-0.016907
10	0.118767	-0.129769	-0.237515	0.086541	0.079075	-0.017382
100	0.118768	-0.129766	-0.237536	0.086511	0.079179	-0.017302

5: The convergence of the first six coefficients in the Hermite polynomial expansion $g(X) = \cos(x)$, where $X \sim \mathcal{N}(\mu = 0.5, \sigma^2 = 4)$ as estimated by different Gauss-Hermite quadrature rules.

Uniform Random Variables

- When the input parameter is not normally distributed, we need a different polynomial expansion to approximate the mapping from input parameter to output random variable.
- Consider a random variable X that is uniformly distributed in the range $[a, b]$.
- In this case we write $X \sim \mathcal{U}[a, b]$.
- The PDF of X is

$$f(x) = \begin{cases} \frac{1}{b-a} & x \in [a, b] \\ 0 & \text{otherwise} \end{cases}. \tag{25}$$

The mean of a uniform distribution is $(b-a)/2$ and the variance is $(b-a)^2/12$.

Uniform Random Variables

- As with normal random variables, it is useful to convert general uniform random variables to a standardized random variable.
- It is more common to think of a standard uniform random variable as having the range $[0,1]$. However, defining the standard to be symmetric about the origin makes for easier algebra down the road.
- We map the interval $[a,b]$ to $[-1,1]$ to correspond with the support with the standard definition of Legendre polynomials.
- If $Z \sim \mathcal{U}[-1,1]$, then

$$x = \frac{b-a}{2}z + \frac{a+b}{2}, \tag{26}$$

  and

$$z = \frac{a+b-2x}{a-b}. \tag{27}$$

- The expectation operator on a uniform random variable transforms to

$$E[g(X)] = \frac{1}{b-a}\int_a^b g(x)\,dx = \frac{1}{2}\int_{-1}^{1} g\left(\frac{b-a}{2}z + \frac{a+b}{2}\right) dz. \tag{28}$$

Legendre Polynomials

- For a function on the range $[-1,1]$ the Legendre polynomials form an orthogonal basis.
- The Legendre polynomials are defined as

$$P_n(x) = \frac{1}{2^n n!} \frac{d^n}{dx^n} \left[(x^2 - 1)^n \right]. \tag{29}$$

- The orthogonality relation for Legendre polynomials is written as

$$\int_{-1}^{1} P_n(x) P_{n'}(x)\, dx = \frac{2}{2n+1} \delta_{nn'}. \tag{30}$$

Legendre Polynomials

n	$P_n(x)$
0	1
1	x
2	$\frac{1}{2}(3x^2 - 1)$
3	$\frac{1}{2}(5x^3 - 3x)$
4	$\frac{1}{8}(35x^4 - 30x^2 + 3)$
5	$\frac{1}{8}(63x^5 - 70x^3 + 15x)$
6	$\frac{1}{16}(231x^6 - 315x^4 + 105x^2 - 5)$
7	$\frac{1}{16}(429x^7 - 693x^5 + 315x^3 - 35x)$
8	$\frac{1}{128}(6435x^8 - 12012x^6 + 6930x^4 - 1260x^2 + 35)$
9	$\frac{1}{128}(12155x^9 - 25740x^7 + 18018x^5 - 4620x^3 + 315x)$
10	$\frac{1}{256}(46189x^{10} - 109395x^8 + 90090x^6 - 30030x^4 + 3465x^2 - 63)$

6: The first ten Legendre polynomials.

Legendre Expansions

The expansion of a square-integrable function on the interval $[a, b]$ in Legendre polynomials is then

$$g(x) = \sum_{n=0}^{\infty} c_n P_n \left(\frac{a+b-2x}{a-b} \right), \qquad x \in [a, b], \tag{31}$$

where c_n is defined by

$$c_n = \frac{2n+1}{2} \int_{-1}^{1} g\left(\frac{b-a}{2} z + \frac{a+b}{2} \right) P_n(z)\, dz. \tag{32}$$

Legendre Expansions

- As before, c_0 will be the mean of the random variable $G \sim g(X)$:

$$c_0 = \frac{1}{2}\int_{-1}^{1} g\left(\frac{b-a}{2}z + \frac{a+b}{2}\right) dz = \frac{1}{b-a}\int_a^b g(x)\,dx = E[G]. \tag{33}$$

- Additionally, the variance of the G is equivalent to the sum of the squares of the coefficients with $n \geq 1$:

$$\mathrm{Var}(G) = \frac{1}{2}\int_{-1}^{1}\left(\sum_{n=0}^{\infty} c_n P_n(z)\right)^2 dz - c_0^2 = \sum_{n=1}^{\infty}\frac{c_n^2}{2n+1}. \tag{34}$$

Legendre Expansion: $g(X) = \cos x$

- For the function $g(X) = \cos(x)$. with $X \sim \mathcal{U}(0, 2\pi)$, we get

$$c_n = \frac{2n+1}{2} \int_{-1}^{1} \cos(\pi z + \pi) P_n(z)\, dz = -\frac{2n+1}{2} \int_{-1}^{1} \cos(\pi z) P_n(z)\, dz. \tag{35}$$

- This makes the expansion, through sixth-order

$$\cos(X) \approx \frac{15}{\pi^2} P_2(z) + \frac{45(4\pi^2 - 42)}{2\pi^4} P_4(z) + \frac{273(7920 - 960\pi^2 + 16\pi^4)}{16\pi^6} P_6(z) \quad X \sim \mathcal{U}(0, 2\pi), \tag{36}$$

and z is related to x via Eq. (27).

$g(X) = \cos x$, convergence of Variance

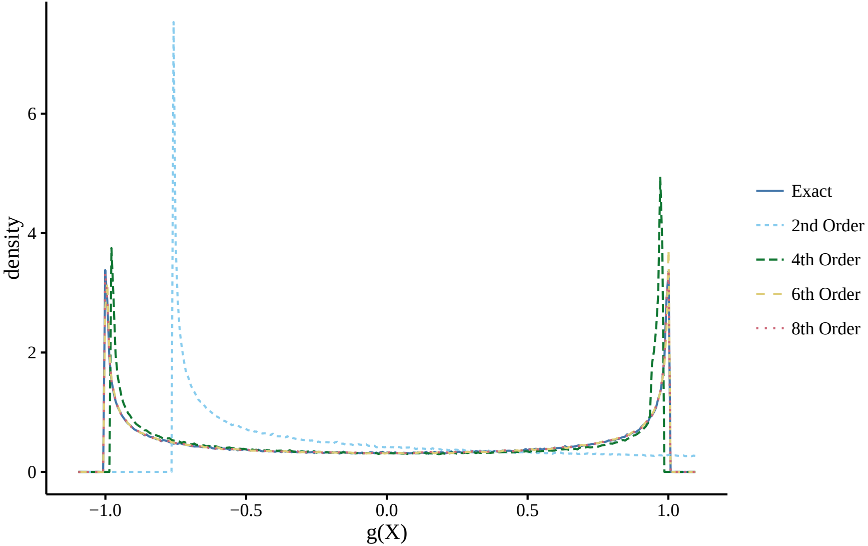
The variance of this function is given by

$$\mathrm{Var}(G) = \frac{1}{2\pi}\int_0^{2\pi} \cos^2(x)\,dx = \frac{1}{2}. \tag{37}$$

order	variance
0	0
2	0.461969
4	0.499663
6	0.499999
8	0.500000
∞	0.500000

7: The convergence of $\mathrm{Var}(G)$ for $g(X) = \cos(x)$, where $X \sim \mathcal{U}(0, 2\pi)$.

$g(X) = \cos x$, Different Expansion Orders



Gauss-Legendre Quadrature

- For estimating the coefficients in a Legendre expansion, Gauss-Legendre quadrature is a natural choice.
- Gauss-Legendre quadrature approximately integrates functions on the range $[-1, 1]$ as

$$\int_{-1}^{1} f(z)\,dz \approx \sum_{i=1}^{n} w_i f(z_i), \tag{38}$$

where the z_i are the roots of P_n,
- The weights are given by

$$w_i = \frac{2}{\left(1 - z_i^2\right)\left[P_n'(z_i)\right]^2}. \tag{39}$$

- Gauss-Legendre quadrature integrates polynomials of degree $2n - 1$ exactly.

Gauss-Legendre Quadrature

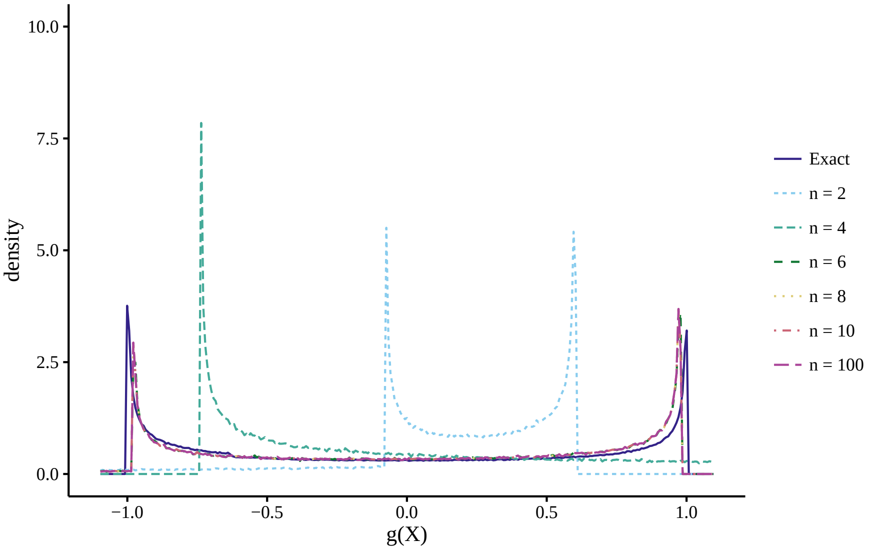
n	$\|x_i\|$	w_i
1	0	2
2	$\frac{1}{\sqrt{3}}$	1
3	0	$\frac{8}{9}$
	$\sqrt{\frac{3}{5}}$	$\frac{5}{9}$
4	0.3399810436	0.652145155
	0.8611363116	0.347854845
	0	0.568888889
5	0.5384693101	0.47862867
	0.9061798459	0.2369268851
	0.2386191860	0.467913935
6	0.6612093865	0.360761573
	0.9324695142	0.171324492

$g(X) = \cos x$, Coefficients for Different Quadrature Rules

n	c_0	c_1	c_2	c_3	c_4	c_5
2	0.240619	0.000000	0.000000	0.000000	-0.842165	0.000000
3	-0.022454	0.000000	1.955092	0.000000	-2.639374	0.000000
4	0.001068	0.000000	1.478399	0.000000	-0.000000	0.000000
5	-0.000031	0.000000	1.521801	0.000000	-0.637516	0.000000
6	0.000001	0.000000	1.519760	0.000000	-0.579819	0.000000
7	0.000000	0.000000	1.519819	0.000000	-0.582523	0.000000
8	0.000000	0.000000	1.519818	0.000000	-0.582445	0.000000
9	0.000000	0.000000	1.519818	0.000000	-0.582447	0.000000
10	0.000000	0.000000	1.519818	0.000000	-0.582447	0.000000
100	0.000000	0.000000	1.519818	0.000000	-0.582447	0.000000

9: The convergence of the first six coefficients in the Legendre polynomial expansion $g(X) = \cos(x)$, where $X \sim \mathcal{U}(0, 2\pi)$ as estimated by Gauss-Legendre quadrature rules using different values of n.

$g(X) = \cos x$, Distributions for Different Quadrature



Beta Random Variables

- A random variable that takes on a value in the range, $[-1,1]$, can often be described by a beta distribution
- A random variable Z that is beta-distributed is written as $Z \sim \mathcal{B}(\alpha,\beta)$, where $\alpha > -1$ and $\beta > -1$ are parameters. The PDF for Z is given by

$$f(z) = \frac{2^{-(\alpha+\beta+1)}}{\alpha+\beta+1}\frac{\Gamma(\alpha+1)+\Gamma(\beta+1)}{\Gamma(\alpha+\beta+1)}(1+z)^{\beta}(1-z)^{\alpha} \qquad z \in [-1,1]. \tag{40}$$

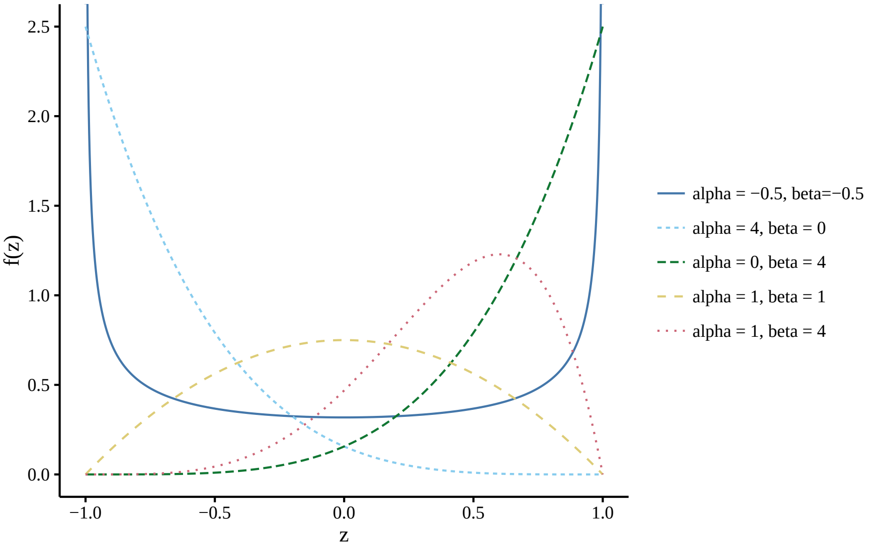
- This is called a beta distribution because the PDF can be expressed in terms of the beta function, $B(\alpha,\beta)$

$$B(\alpha,\beta) = \frac{\Gamma(\alpha)\Gamma(\beta)}{\Gamma(\alpha+\beta)}, \tag{41}$$

as

$$f(z) = \frac{2^{-(\alpha+\beta+1)}}{B(\alpha+1,\beta+1)}(1+z)^{\beta}(1-z)^{\alpha} \qquad z \in [-1,1]. \tag{42}$$

Beta Random Variables



A Note of Caution on the Beta Distribution

- There is some subtlety regarding the support of $\mathbf{z}$.
- If α or β is less than 0 then one or both of the endpoints is excluded due to a singularity.
- The definition of the beta distribution used here is not the typical statistician's distribution.
- The statistician's distribution has support on $[0,1]$ and uses parameters α' and β' that are equal to

$$\alpha' = \alpha + 1 \qquad \beta' = \beta + 1$$

.

- As we will see, our definition is well-suited to expansion in Jacobi polynomials.

Beta Random Variables

- We can scale the distribution to a general range $X \in [a, b]$ using Eqs. (26) and (27).
- The expectation operator in this case is given by

$$E[g(X)] = \int_{-1}^{1} g\left(\frac{b-a}{2}z + \frac{a+b}{2}\right) \frac{2^{-(\alpha+\beta+1)}(1+z)^{\beta}(1-z)^{\alpha}}{B(\alpha+1, \beta+1)} dz. \tag{43}$$

- From this we get following for a beta distribution on the range $[a, b]$:

$$\bar{x} = \frac{(\alpha+1)a + (\beta+1)b}{\alpha+\beta+2}, \qquad \mathrm{Var}(X) = \frac{(\alpha+1)(\beta+1)(a-b)^2}{(\alpha+\beta+2)^2(\alpha+\beta+3)}. \tag{44}$$

Jacobi Polynomials

- The Jacobi polynomials, $P_n^{(\alpha,\beta)}(z)$ are orthogonal polynomials under the weight $(1-z)^\alpha(1+z)^\beta$ for the interval $z \in [-1,1]$.
- These polynomials can be defined in several ways, including Rodrigues' formula:

$$P_n^{(\alpha,\beta)}(z) = \frac{(-1)^n}{2^n n!}(1-z)^{-\alpha}(1+z)^{-\beta}\frac{d^n}{dz^n}\left\{(1-z)^\alpha(1+z)^\beta\left(1-z^2\right)^n\right\} \tag{45}$$

- When $\alpha = \beta = 0$ these polynomials are the Legendre polynomials.
- These polynomials have the, somewhat ugly, orthogonality relation

$$\langle P_m^{(\alpha,\beta)}(z)P_n^{(\alpha,\beta)}(z)\rangle = \frac{2^{\alpha+\beta+1}}{2n+\alpha+\beta+1}\frac{\Gamma(n+\alpha+1)\Gamma(n+\beta+1)}{\Gamma(n+\alpha+\beta+1)n!}\delta_{nm}, \tag{46}$$

where

$$\langle g(z), h(z)\rangle = \int_{-1}^{1}(1-z)^\alpha(1+z)^\beta g(z)h(z)\,dz. \tag{47}$$

Jacobi Polynomials

n	$P_n^{(\alpha,\beta)}(z)$
0	1
1	$\frac{1}{2}(\alpha-\beta+z(\alpha+\beta+2))$
2	$\frac{1}{2}(\alpha+1)(\alpha+2)+\frac{1}{8}(z-1)^2(\alpha+\beta+3)(\alpha+\beta+4)+\frac{1}{2}(z-1)(\alpha+2)(\alpha+\beta+3)$
3	$\frac{1}{6}(\alpha+1)(\alpha+2)(\alpha+3)+\frac{1}{48}(z-1)^3(\alpha+\beta+4)(\alpha+\beta+5)(\alpha+\beta+6)+$
	$+\frac{1}{8}(z-1)^2(\alpha+3)(\alpha+\beta+4)(\alpha+\beta+5)+\frac{1}{4}(z-1)(\alpha+2)(\alpha+3)(\alpha+\beta+4)$

10: The first three Jacobi polynomials.

Jacobi Expansions

A function that is square-integrable with respect to the inner product in Eq. (47) can be written as

$$g(x) = \sum_{n=0}^{\infty} c_n P_n^{(\alpha,\beta)}\left(\frac{a+b-2x}{a-b}\right), \qquad x \in [a,b], \tag{48}$$

where the constant is defined as

$$c_n = \langle P_n^{(\alpha,\beta)}(z) P_n^{(\alpha,\beta)}(z)\rangle^{-1} \int_{-1}^{1} g\left(\frac{b-a}{2} z + \frac{a+b}{2}\right) P_n^{(\alpha,\beta)}(z)(1-z)^{\alpha}(1+z)^{\beta}\, dz. \tag{49}$$

Jacobi Expansions

- It is worthwhile to look at c_0, i.e., the mean (expected value) of $G \sim g(X)$:

$$c_0 = \frac{2^{-(\alpha+\beta+1)}}{B(\alpha+1,\beta+1)} \int_{-1}^{1} g\left(\frac{b-a}{2}z + \frac{a+b}{2}\right)(1-z)^{\alpha}(1+z)^{\beta}\,dz = E[g(X)]. \tag{50}$$

- Also, by construction the variance in $g(X)$ is the sum of the squares of the c_n for $n > 0$:

$$\mathrm{Var}(G) = E[g^2(X)] - (E[g(X)])^2 = \frac{2^{-(\alpha+\beta+1)}}{B(\alpha+1,\beta+1)} \sum_{n=1}^{\infty} c_n^2 \langle P_n^{(\alpha,\beta)}(z) P_n^{(\alpha,\beta)}(z)\rangle. \tag{51}$$

Jacobi Expansions: $g(X) = \cos X$

- Consider $g(X) = \cos(x)$, where $X \in [0, 2\pi]$ and X is derived from a standard beta random variable $Z \sim \mathcal{B}(4,1)$:

$$c_n = \langle P_n^{(\alpha,\beta)}(z) P_n^{(\alpha,\beta)}(z) \rangle^{-1} \int_{-1}^{1} \cos(\pi z + \pi) P_n^{(4,1)}(z)\, dz. \qquad (52)$$

- The mean value of $G \sim \cos(X)$ is

$$c_0 = -\frac{15(\pi^2 - 9)}{2\pi^4} \approx -0.0669551. \qquad (53)$$

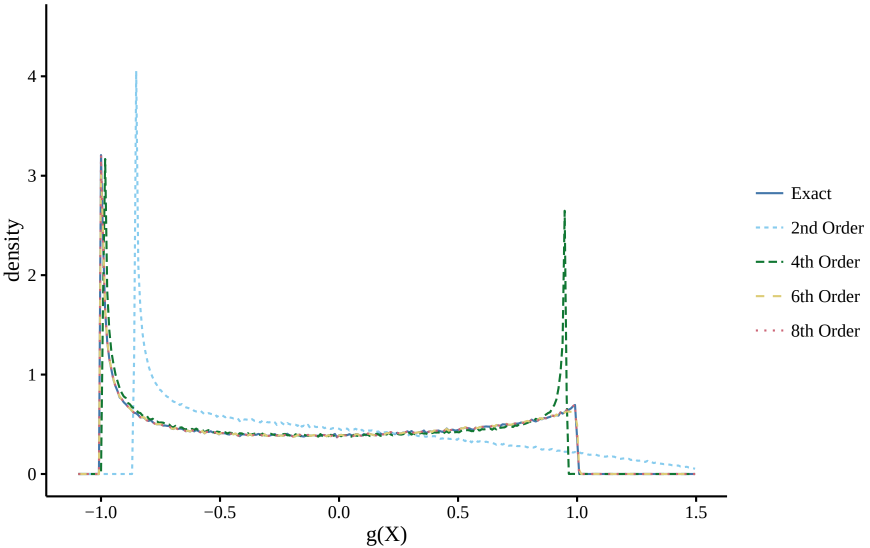
- The expansion, through third-order is

$$\cos(X) \approx -\frac{15(\pi^2-9)}{2\pi^4} + \frac{6(315 - 60\pi^2 + 2\pi^4)}{\pi^6} P_1^{(4,1)}(z) - \frac{35(630 - 75}{2\pi^6}$$
$$+ \frac{12(-51975 + 8190\pi^2 - 315\pi^4 + 2\pi^6)}{\pi^8} P_3^{(4,1)}(z) \quad Z \sim \mathcal{B}(4,1), \qquad (54)$$

or

$$\cos(X) \approx 2.50342 z^3 + 4.14706 z^2 - 0.536325 z - 1.00484 \quad Z \sim \mathcal{B}(4,1).$$

Jacobi Expansions: $g(X) = \cos X$



Jacobi Expansions: $g(X) = \cos X$

The variance of G is given by

$$\mathrm{Var}(G) = \frac{2^{-(\alpha+\beta+1)}}{B(\alpha+1,\beta+1)} \int_{-1}^{1} \cos^2(\pi z + \pi)(1-z)^{\alpha}(1+z)^{\beta}\,dz - \left(\frac{15\left(\pi^2-9\right)}{2\pi^4}\right)^2 \tag{55}$$

$$= \frac{1}{64}\left(\frac{135}{\pi^4} + 32 - \frac{60}{\pi^2}\right) - \frac{225\left(\pi^2-9\right)^2}{4\pi^8} \approx 0.4221832.$$

Notice that at fourth-order the estimate is correct to three digits.

order	variance
1	0.3302376
2	0.4001581
4	0.4220198
6	0.4221829
8	0.4221832
∞	0.4221832

11: Convergence of $\mathrm{Var}(G)$ for $g(X) = \cos(x)$, $x = \pi z + \pi$ and $Z \sim \mathcal{B}(4,1)$.

Gauss-Jacobi Quadrature

- To estimate the integrals required to compute a Jacobi expansion of a function of a beta-distributed random variables, we turn to Gauss-Jacobi quadrature.
- As in Gauss-Legendre quadrature (recall that Legendre polynomials are a special case of Jacobi polynomials), the quadrature rule looks like

$$\int_{-1}^{1} f(z)(1-z)^{\alpha}(1+z)^{\beta}\,dz \approx \sum_{i=1}^{n} w_i f(z_i). \tag{56}$$

- The abscissas, z_i, for the quadrature rule are the n roots of $P_n^{(\alpha,\beta)}(z)$, and the weights are given by

$$w_i = \frac{2n+\alpha+\beta+2}{n+\alpha+\beta+1}\frac{\Gamma(n+\alpha+1)\Gamma(n+\beta+1)}{\Gamma(n+\alpha+\beta+1)(n+1)!}\frac{2^{\alpha+\beta}}{P_n'^{(\alpha,\beta)}(z_i)P_{n+1}^{(\alpha,\beta)}(z_i)}, \tag{57}$$

Gauss-Jacobi Quadrature

- Here, unlike in Gauss-Legendre quadrature, the weights and abscissas depend on the choice of α and β. Therefore, we will not give an extensive table of coefficients because the generality makes the formulas lengthy. The first-order quadrature ($n = 1$) is

$$x_1 = \frac{b - a}{a + b + 2}, \qquad w_1 = \frac{2^{a+b+1}\Gamma(a+2)\Gamma(b+2)}{(a+1)(b+1)\Gamma(a+b+2)}. \tag{58}$$

- Beyond $n = 1$ the formulas for the weights and abscissas will not fit on a page, so they do not appear here.

Gauss-Jacobi Quadrature, for $\mathcal{B}(4,1)$

- For $Z \sim \mathcal{B}(4,1)$, the quadrature rules are given in below.
- Notice that unlike Gauss-Legendre quadrature rules, these rules are not symmetric about the origin.
- Moreover, the weights sum to the integral of the weight function over the domain:

$$\sum_{i=1}^{n} w_i = \int_{-1}^{1} (1-z)^4 (1+z)\, dz = \frac{32}{15}. \tag{59}$$

Gauss-Jacobi Quadrature, for $\mathcal{B}(4,1)$

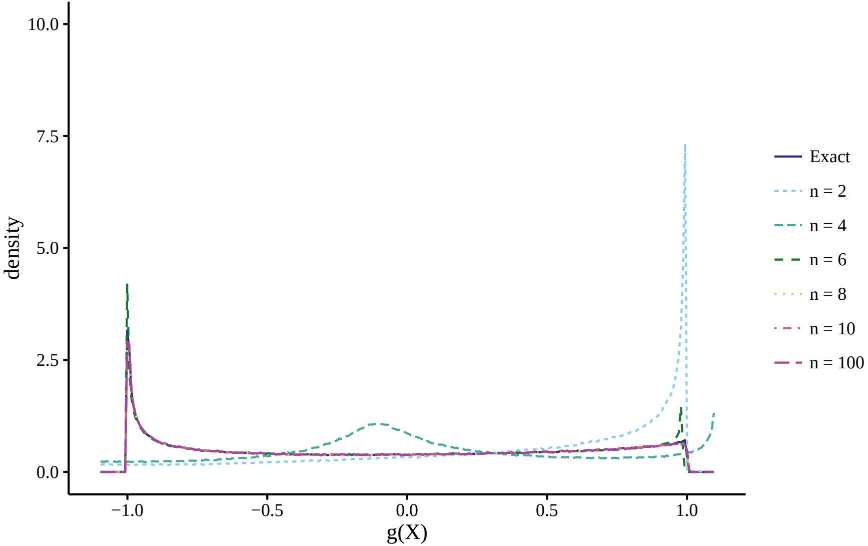
n	z_i	w_i
1	$-\frac{3}{7}$	$\frac{32}{15}$
2	0	$\frac{16}{21}$
	$-\frac{2}{3}$	$\frac{48}{35}$
	0.273378	0.213558
3	-0.313373	1.121472
	-0.778187	0.798303
	0.451910	0.062182
4	-0.037021	0.545298
	-0.497091	1.049649
	-0.840875	0.476204
	0.573288	0.019805
	0.169240	0.233970
5	-0.247188	0.732908
	-0.615377	0.850154
	-0.879964	0.296496

$g(X) = \cos x$, Coefficients for Different Quadrature Rules

n	c_0	c_1	c_2	c_3	c_4	c_5
2	-0.035714	-0.642857	0.000000	0.589286	-0.157292	-0.259369
3	-0.069292	-0.503277	0.282089	0.000000	-0.280037	0.478186
4	-0.066861	-0.514456	0.229440	0.132105	-0.000000	-0.135492
5	-0.066957	-0.513982	0.233355	0.120895	-0.058189	0.000000
6	-0.066955	-0.513994	0.233197	0.121391	-0.053616	-0.011632
7	-0.066955	-0.513994	0.233201	0.121378	-0.053807	-0.011110
8	-0.066955	-0.513994	0.233201	0.121378	-0.053802	-0.011124
9	-0.066955	-0.513994	0.233201	0.121378	-0.053802	-0.011124
10	-0.066955	-0.513994	0.233201	0.121378	-0.053802	-0.011124
100	-0.066955	-0.513994	0.233201	0.121378	-0.053802	-0.011124

12: The convergence of the first six coefficients in the Jacobi polynomial expansion $g(X) = \cos(x)$, where $x = \pi z + \pi$ and $Z \sim \mathcal{B}(4, 1)$ as estimated by Gauss-Jacobi quadrature rules using different values of n.

$g(X) = \cos x$, Distributions for Different Quadrature



Gamma Random Variables

- The final class of random variable we will consider are gamma random variables.
- These random variables have support on $(0, \infty)$
- When X is a gamma-distributed random variable we will write $X \sim \mathcal{G}(\alpha, \beta)$ where the PDF of the random variable is

$$f(X) = \frac{\beta^{(\alpha+1)} x^{\alpha} e^{-\beta x}}{\Gamma(\alpha+1)}, \qquad x \in (0, \infty), \quad \alpha > -1, \, \beta > 0. \tag{60}$$

- The distribution gets its name from the appearance of the gamma function in the PDF.
- There are several definitions of gamma random variables. One common definition has a different parameter $\alpha' = \alpha + 1$, but the same parameter β.

Gamma Random Variables

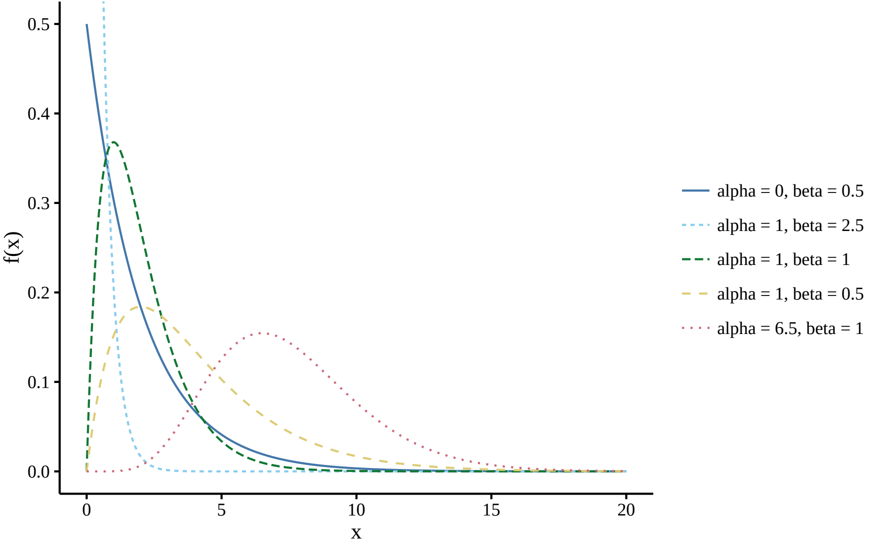
- As in other variables, it will be useful to have a standardized gamma random variable.
- In this case we define a $Z \sim \mathcal{G}(\alpha, 1)$, so that Z has the PDF

$$f(z) = \frac{z^{\alpha} e^{-z}}{\Gamma(\alpha + 1)}, \qquad z \in (0, \infty), \quad \alpha > -1. \tag{61}$$

- We can change from Z to X using a simple scaling

$$z = \beta x. \tag{62}$$

Gamma Random Variables



α moves the peak of the distribution and that β, as we mentioned above, scales the distribution.

Gamma Random Variables

- The expectation operator for a gamma random variable can be written as

$$E[g(X)] = \int_0^\infty g(x) \frac{\beta^{(\alpha+1)} x^\alpha e^{-\beta x}}{\Gamma(\alpha+1)} dx = \int_0^\infty g\left(\frac{z}{\beta}\right) \frac{z^\alpha e^{-z}}{\Gamma(\alpha+1)} dz. \quad (63)$$

- Additionally, the mean and variance are given by

$$\bar{x} = \frac{\alpha+1}{\beta}, \qquad \mathrm{Var}(X) = \frac{\alpha+1}{\beta}. \quad (64)$$

Laguerre Polynomials

- The orthogonal polynomials that we will use with functions of a gamma random variable are generalized Laguerre polynomials.
- Rodrigues' formula for these polynomials is

$$L_n^{(\alpha)}(x) = \frac{x^{-\alpha} e^x}{n!} \frac{d^n}{dx^n} \left(e^{-x} x^{n+\alpha} \right). \tag{65}$$

n	$L_n^{(\alpha)}(z)$
0	1
1	$\alpha - x + 1$
2	$\frac{1}{2}\left(\alpha^2 + 3\alpha + x^2 - 2\alpha x - 4x + 2\right)$
3	$\frac{1}{6}\left(\alpha^3 + 6\alpha^2 + 11\alpha - x^3 + 3\alpha x^2 + 9x^2 - 3\alpha^2 x - 15\alpha x - 18x + 6\right)$

13: The first three generalized Laguerre polynomials.

Laguerre Polynomials

- The generalized Laguerre polynomials have the following orthogonality condition

$$\int_0^\infty x^\alpha e^{-x} L_n^{(\alpha)}(x) L_m^{(\alpha)}(x)\,dx = \frac{\Gamma(n+\alpha+1)}{n!}\delta_{n,m}. \tag{66}$$

- The generalized Laguerre polynomials form a basis for functions on $(0,\infty)$ that are square integrable with the inner product

$$\langle g(z), h(z) \rangle = \int_0^\infty z^\alpha e^{-z} g(z) h(z)\,dz. \tag{67}$$

- We can write a function $g(X)$ where $X \sim \mathcal{G}(\alpha, \beta)$ using the following expansion

$$g(x) = \sum_{n=0}^{\infty} c_n L_n^{(\alpha)}(\beta x), \tag{68}$$

where the expansion coefficients are

$$c_n = \frac{n!}{\Gamma(n+\alpha+1)} \int_0^\infty g\left(\frac{z}{\beta}\right) z^\alpha e^{-z} L_n^{(\alpha)}(z)\,dz. \tag{69}$$

Laguerre Polynomials

- The value of c_0 is once again the mean of $G \sim g(X)$ where $X \sim \mathcal{G}(\alpha, \beta)$:

$$c_0 = \int_0^\infty g\left(\frac{z}{\beta}\right) \frac{z^\alpha e^{-z}}{\Gamma(\alpha+1)} dz = E[g(X)]. \tag{70}$$

- The variance of G is related to the sum of the squares of the expansion coefficients:

$$\begin{aligned} \mathrm{Var}(G) &= \int_0^\infty \left(\sum_{n=0}^\infty c_n L_n^{(\alpha)}(z) \right)^2 \frac{z^\alpha e^{-z}}{\Gamma(\alpha+1)} dz - c_0^2 \\ &= \sum_{n=1}^\infty \frac{\Gamma(n+\alpha+1)}{\Gamma(\alpha+1) n!} c_n^2. \end{aligned} \tag{71}$$

Laguerre Polynomials: $g(X) = \cos x$

- When $g(x) = \cos x$ and $X \sim \mathcal{G}(1,2)$, the expansion coefficients are given by

$$c_n = \frac{n!}{\Gamma(n+2)} \int_0^\infty \cos\left(\frac{z}{2}\right) z e^{-z} L_n^{(1)}(z)\, dz. \tag{72}$$

- The expected value of G is

$$c_0 = \int_0^\infty \cos\left(\frac{z}{2}\right) z e^{-z}\, dz = \frac{12}{25}. \tag{73}$$

- The expansion to third-order is

$$\cos(X) \approx \frac{12}{25} + \frac{44}{125}(2-2x) + \frac{28}{625}(2x^2-6x+3) + \frac{656}{9375}(x^3-6x^2+9x-3) \quad X \sim \mathcal{G}(1,2). \tag{74}$$

Laguerre Polynomials: $g(X) = \cos x$

- The variance of G is given by

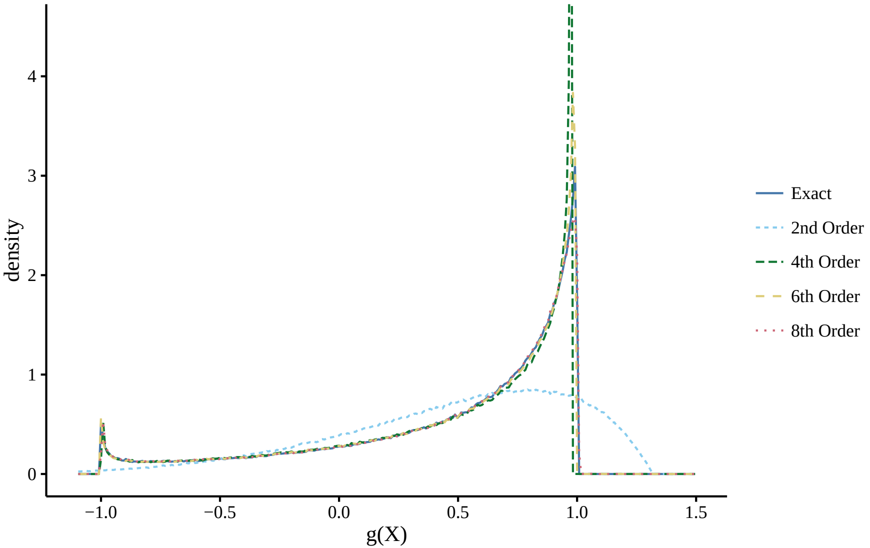
$$\mathrm{Var}(G) = \sum_{n=1}^{\infty} \frac{\Gamma(n+2)}{\Gamma(2)n!} c_n^2 = \frac{337}{1250} = 0.2696. \qquad (75)$$

- The variance is well-estimated by the fourth-order expansion. We will also see that the fourth-order expansion is also a good estimate of the distribution of G.

order	variance
1	0.2478080
2	0.2538291
4	0.2693313
6	0.2695484
8	0.2695967
∞	0.2696000

14: The convergence of $\mathrm{Var}(G)$ for $g(X) = \cos(x)$, where $X \sim \mathcal{G}(1,2)$.

Laguerre Polynomials: $g(X) = \cos x$



Gauss-Laguerre Quadrature

- We turn to generalized Gauss-Laguerre quadrature. The quadrature rule has the form

$$\int_0^\infty f(z) z^\alpha e^{-z} dz \approx \sum_{i=1}^n w_i f(z_i). \tag{76}$$

- The abscissas, z_i, for the quadrature rule are the n roots of $L_n^{(\alpha)}(z)$, and the weights are given by

$$w_i = \frac{\Gamma(n+\alpha) z_i}{n!(n+\alpha)(L_{n-1}^\alpha(z_i))^2}. \tag{77}$$

- The first-order quadrature ($n = 1$) is

$$x_1 = 1 + \alpha, \qquad w_1 = \frac{(\alpha+1)\Gamma(a+1)}{a+1}. \tag{78}$$

For $n = 2$ we have

$$x_{1,2} = \alpha \pm \sqrt{\alpha + 2}, \qquad w_{1,2} = \frac{\left(3 \pm \sqrt{3}\right)\Gamma(a+2)}{2(a+2)\left(a+1-\left(3 \pm \sqrt{3}\right)\right)^2}. \tag{79}$$

Gauss-Laguerre Quadrature

- We turn to generalized Gauss-Laguerre quadrature. The quadrature rule has the form

$$\int_0^\infty f(z) z^\alpha e^{-z}\, dz \approx \sum_{i=1}^{n} w_i f(z_i). \tag{80}$$

- The abscissas, z_i, for the quadrature rule are the n roots of $L_n^{(\alpha)}(z)$, and the weights are given by

$$w_i = \frac{\Gamma(n+\alpha) z_i}{n!(n+\alpha)(L_{n-1}^{\alpha}(z_i))^2}. \tag{81}$$

- The first-order quadrature ($n = 1$) is

$$x_1 = 1 + \alpha, \qquad w_1 = \frac{(\alpha+1)\Gamma(a+1)}{a+1}. \tag{82}$$

For $n = 2$ we have

$$x_{1,2} = \alpha \pm \sqrt{\alpha+2}, \qquad w_{1,2} = \frac{\left(3 \pm \sqrt{3}\right)\Gamma(a+2)}{2(a+2)\left(a+1-\left(3 \pm \sqrt{3}\right)\right)^2}. \tag{83}$$

Gauss-Laguerre Quadrature: $\mathcal{G}(1,2)$

For our example from above, where $X \sim \mathcal{G}(1,2)$, the quadrature rules are given in Table 15. In this case the weights sum to the integral of the weight function over the domain:

$$\sum_{i=1}^{n} w_i = \int_0^\infty z e^{-z} dz = 2. \tag{84}$$

Gauss-Laguerre Quadrature: $\mathcal{G}(1,2)$

n	z_i	w_i
1	2	1
2	$3 \pm \sqrt{3}$	$\frac{3\pm\sqrt{3}}{3\left(2-\left(3\pm\sqrt{3}\right)\right)^2}$
3	7.758770 3.305407 0.935822	0.020102 0.391216 0.588681
4	10.953894 5.731179 2.571635 0.743292	0.001316 0.074178 0.477636 0.446871
5	14.260103 8.399067 4.610833 2.112966 0.617031	0.000069 0.008720 0.140916 0.502281 0.348015

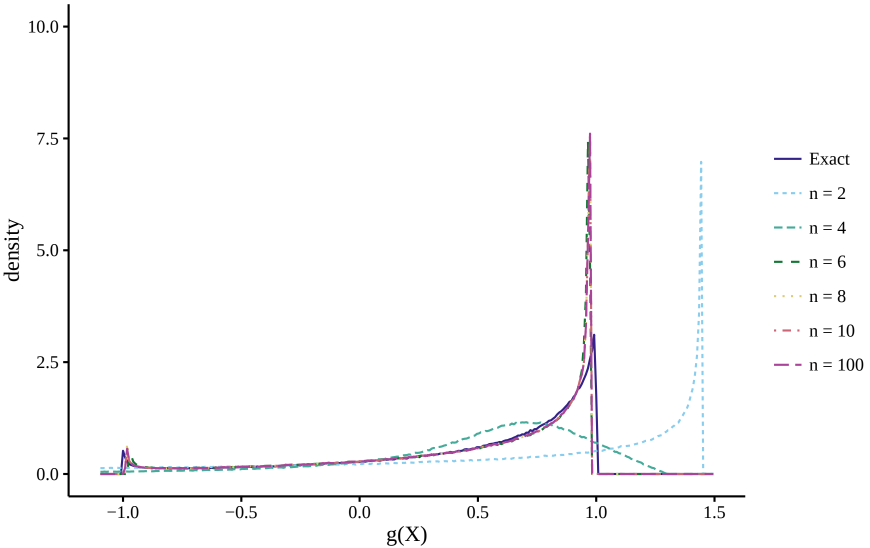
15: The abscissas and weights for generalized Gauss-Laguerre quadrature up to order 5 with $\alpha = 1$.

$g(X) = \cos x$, Coefficients for Different Quadrature Rules

n	c_0	c_1	c_2	c_3	c_4	c_5
2	0.484528	0.438701	0.000000	-0.219350	-0.223933	-0.140776
3	0.478523	0.343285	0.077209	-0.000000	-0.046325	-0.099540
4	0.480185	0.352313	0.038293	-0.054229	-0.000000	0.036153
5	0.479984	0.352043	0.045559	-0.053931	-0.036908	-0.000000
6	0.480001	0.351990	0.044746	-0.052110	-0.029267	-0.004078
7	0.480000	0.352001	0.044801	-0.052532	-0.029939	-0.000867
8	0.480000	0.352000	0.044800	-0.052475	-0.029968	-0.001564
9	0.480000	0.352000	0.044800	-0.052480	-0.029949	-0.001480
10	0.480000	0.352000	0.044800	-0.052480	-0.029952	-0.001484
100	0.480000	0.352000	0.044800	-0.052480	-0.029952	-0.001485

16: The convergence of the first six coefficients in the generalized Laguerre polynomial expansion $g(X) = \cos(x)$, where $X \sim \mathcal{G}(1,2)$ as estimated by generalized Gauss-Laguerre quadrature rules using different values of n.

$g(X) = \cos x$, Distributions for Different Quadrature



Intermission

We have reviewed

- Why uncertainty quantification is important,
- Why we want to minimize the number of times we need to perform a simulation,
- How to estimate quantities of interest with Monte Carlo (and why that might not be a great idea),
- How to approximate a distribution using polynomial expansions in probability space depending on the underlying distribution.

Next we will

- Show results for more interesting problems,
- Discuss how this works for multiple input random variables,
- Explore how to minimize the number of function evaluations needed.

Thank you!

Polynomial Chaos Expansions for Uncertainty Quantification

AICES EU Regional School 2016 - Part 1

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