Numerical Optimization 17: Uncertainty

Qiang Zhu

University of Nevada Las Vegas

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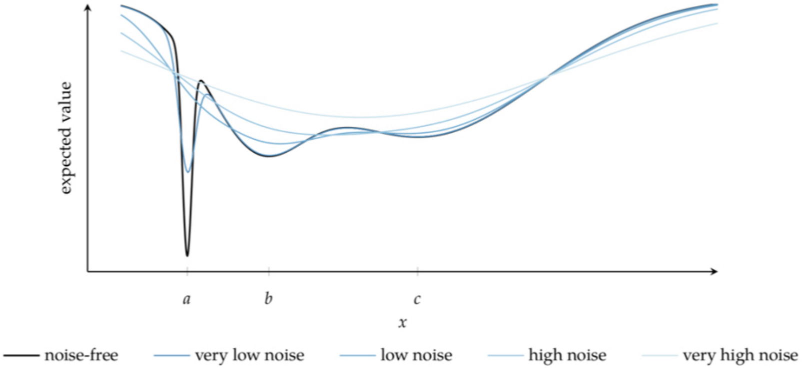
Overview

Uncertainty

In many engineering tasks, however, there may be uncertainty due to a number of factors, such as model approximations, imprecision, and fluctuations of parameters over time. We want to minimize $f(x, z)$, but we do not have control over z. Feasibility depends on both the design vector x and the uncertain vector z.



Polynomial chaos

Polynomial chaos is a method for fitting a polynomial to $f(x, z)$ and using the resulting surrogate model to estimate the mean and variance.
In one dimension, we approximate $f(z)$ with a surrogate model consisting of k polynomial basis functions, $b_1, \cdots, b_k$:

$$f(z) = \hat{f}(z) = \sum_{i=1}^{k} \theta_i b_i(z)$$

The mean of $\hat{f}$ can be derived as follows

$$\begin{aligned} \hat{\mu} &= \int_Z p(z)\hat{f}(z)dz = \int_Z \sum_{i=1}^{k} p(z)\theta_i b_i(z)dx = \sum_{i=1}^{k} \int_Z \theta_i b_i(z)p(z)dz \\ &= \theta_1 \int_Z b_1(z)p(z)dz + \cdots + \theta_n \int_Z b_n(z)p(z)dz \end{aligned}$$

Polynomial chaos

The variance of $\hat{f}$ can be derived as follows

$$
\begin{aligned}
\hat{\sigma} &= \mathbb{E}[\hat{f}^2] - (\mathbb{E}[\hat{f}])^2 = \int_Z p^2(z)\hat{f}(z)dz - \mu^2 \\
&= \int_Z \sum_{i=1}^{k} \sum_{j=1}^{k} \theta_i \theta_j b_i(z) b_j(z) p(z) dz - \mu^2 \\
&= \int_Z \left(\sum_{i=1}^{k} \theta_i^2 b_i^2(z) + 2 \sum_{i=2}^{k} \sum_{j=1}^{i-1} \theta_i \theta_j b_i(z) b_j(z) \right) p(z) dz - \mu^2 \\
&= \sum_{i=1}^{k} \theta_i^2 \int_Z b_i^2(z) dz + 2 \sum_{i=2}^{k} \sum_{j=1}^{i-1} \theta_i \theta_j \int_Z b_i(z) b_j(z) p(z) dz - \mu^2
\end{aligned}
$$

Orthogonal polynomial basis

The mean and variance can be efficiently computed if the basis functions are chosen to be orthogonal under p. Two basis functions b_i and b_j are orthogonal with respect to a probability density $p(z)$ if

$$\int_Z b_i(z)b_j(z)p(z)dz = 0. \text{ (if } i \neq j)$$

If the chosen basis functions are all orthogonal to one another and the first basis function is $b_1(z) = 1$, the mean is:

$$\begin{aligned}\hat{\mu} &= \theta_1 \int_Z b_1(z)p(z)dz + \cdots + \theta_n \int_Z b_n(z)p(z)dz \\ &= \theta_1 \int_Z b_1^2(z)p(z)dz + \cdots + \theta_n \int_Z b_1(z)b_n(z)p(z)dz \\ &= \theta_1\end{aligned}$$

Orthogonal polynomial basis

Similarly, the variance is

$$
\begin{aligned}
\hat{\sigma} &= \sum_{i=1}^{k} \theta_i^2 \int_Z b_i^2(z)dz + 2\sum_{i=2}^{k}\sum_{j=1}^{i-1} \theta_i\theta_j \int_Z b_i(z)b_j(z)p(z)dz - \mu^2 \\
&= \sum_{i=1}^{k} \theta_i^2 \int_Z b_i^2(z)dz - \mu^2 \\
&= \theta_1^2 \int_Z b_1^2(z)dz - \sum_{i=1}^{k} \theta_i^2 \int_Z b_i^2(z)dz - \mu^2 \\
&= \sum_{i=1}^{k} \theta_i^2 \int_Z b_i^2(z)dz
\end{aligned}
$$

Orthogonal polynomial basis

The mean thus falls immediately from fitting a surrogate model to the observed data, and the variance can be very efficiently computed given the values $\int_Z b_i^2(z)p(z)dz$ for a choice of basis functions and probability distribution. All orthogonal polynomials satisfy the recurrence relation:

$$b_{i+1}(z) = \begin{cases} (z - a_i)b_i(z) & i = 1 \\ (z - a_i)b_i(z) - \beta_i b_{i-1} z & \text{else} \end{cases}$$

with $b_1(z) = 1$ and weights

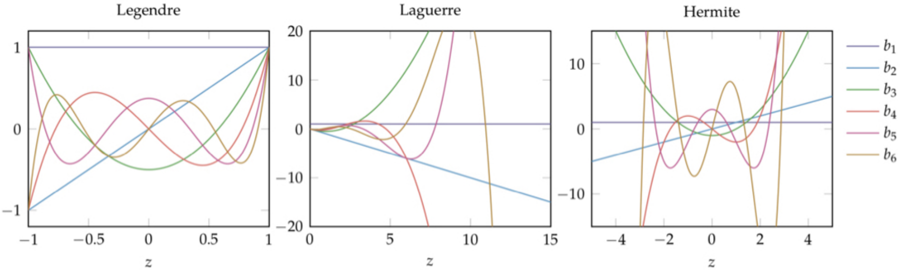
$$\alpha_i = \frac{\int_Z z b_i^2(z)p(z)dz}{\int_Z b_i^2(z)p(z)dz}$$

$$\beta_i = \frac{\int_Z b_i^2(z)p(z)dz}{\int_Z b_{i-1}^2(z)p(z)dz}$$

The recurrence relation can be used to generate the basis functions. Each basis function b_i is a polynomial of degree $i - 1$.

Orthogonal polynomial basis functions

Distribution	Domain	Density	Name	Recursive Form	Closed Form
Uniform	$[-1,1]$	$\frac{1}{2}$	Legendre	$\mathrm{Le}_k(x) = \frac{1}{2^k k!}\frac{d^k}{dx^k}\left[\left(x^2-1\right)^k\right]$	$b_i(x) = \sum_{j=0}^{i-1}\binom{i-1}{j}\binom{-i-2}{j}\left(\frac{1-x}{2}\right)^j$
Exponential	$[0,\infty)$	e^{-x}	Laguerre	$\frac{d}{dx}\mathrm{La}_k(x) = \left(\frac{d}{dx}-1\right)\mathrm{La}_{k-1}$	$b_i(x) = \sum_{j=0}^{i-1}\binom{i-1}{j}\frac{(-1)^j}{j!}x^j$
Unit Gaussian	$(-\infty,\infty)$	$\frac{1}{\sqrt{2\pi}}e^{-x^2/2}$	Hermite	$\mathrm{H}_k(x) = x\mathrm{H}_{k-1} - \frac{d}{dx}\mathrm{H}_{k-1}$	$b_i(x) = \sum_{j=0}^{\lfloor(i-1)/2\rfloor}(i-1)!\frac{(-1)^{\frac{i-1}{2}-j}}{(2j)!(\frac{i-1}{2}-j)!}(2x)^{2j}$



Coefficients

The coefficients $\theta_1, \cdots, \theta_k$ can be inferred by exploiting the orthogonality of the basis functions, producing an integration term amenable to Gaussian quadrature.

$$f(z) = \sum_{i=1}^{k} \theta_i b_i(z)$$

$$\begin{aligned}
\int_Z f(z) b_j(z) p(z) dz &= \int_Z \left(\sum_{i=1}^{k} \theta_i b_i(z) \right) b_j(z) p(z) dz \\
&= \sum_{i=1}^{k} \theta_i \int_Z b_i(z) b_j(z) p(z) dz \\
&= \theta_j \int_Z b_j(z) p(z) dz \\
\implies \theta_j &= \frac{\int_Z f(z) b_j(z) p(z) dz}{\int_Z b_j(z) p(z) dz}
\end{aligned}$$

Multivariate

Polynomial chaos can be applied to functions with multiple random inputs. Multivariate basis functions over m variables are constructed as a product over univariate orthogonal polynomials:

Summary

- Polynomial chaos is a powerful uncertainty propagation technique basedon orthogonal polynomials.
- Bayesian Monte Carlo uses Gaussian processes to efficiently arrive at the moments with analytic results for Gaussian kernels.