MANUAL

INL/EXT-19-53843
Revision 0
Printed April 2019

RAVEN Analytic Test Documentation

Andrea Alfonsi, Paul W. Talbot, Diego Mandelli, Congjian Wang, Joshua Cogliati, Cristian Rabiti

Prepared by
Idaho National Laboratory
Idaho Falls, Idaho 83415

The Idaho National Laboratory is a multiprogram laboratory operated by
Battelle Energy Alliance for the United States Department of Energy
under DOE Idaho Operations Office. Contract DE-AC07-05ID14517.

Approved for unlimited release.

Issued by the Idaho National Laboratory, operated for the United States Department of Energy by Battelle Energy Alliance.

Printed in the United States of America. This report has been reproduced directly from the best available copy.

INL/EXT-19-53843
Revision 0
Printed April 2019

RAVEN Analytic Test Documentation

Andrea Alfonsi
Paul W. Talbot
Congjian Wang
Diego Mandelli
Joshua Cogliati
Cristian Rabiti

Contents

1 Introduction

In the interest of benchmarking and maintaining algorithms developed and used within `raven`, we present here analytic benchmarks associated with specific models. The associated external models referenced in each case can be found in

```
raven/tests/framework/AnalyticModels/
```

2 Projectile (vacuum, gravity)

Associated external model: `projectile.py`

Solves the projectile motion equations

$$x = x_0 + v_{x,0}t, \tag{1}$$

$$y = y_0 + v_{y,0}t + \frac{a}{2}t^2, \tag{2}$$

with the following inputs

- x_0, or `x0`, initial horizontal position,
- y_0, or `y0`, initial vertical position,
- v_0, or `v0`, initial speed (scalar),
- θ, or `ang`, angle with respect to horizontal plane,

and following responses:

- r, or `r`, the horizontal distance traveled before hitting $y = 0$,
- x, or `x`, the time-dependent horizontal position,
- y, or `y`, the time-dependent vertical position,
- t, or `time`, the series of time steps taken.

The simulation takes 10 equally spaced time steps from 0 to 1 second, inclusive, and returns all four values as vector quantities.

2.1 Grid, x_0, y_0

If a Grid sampling strategy is used and the following distributions are applied to x_0 and y_0, with three samples equally spaced on the CDF between 0.01 and 0.99 for each input, the following are some of the samples obtained.

- x_0 is distributed normally with mean 0 and standard deviation 1,
- y_0 is distributed normally with mean 1 and standard deviation 0.2.

x_0	y_0	t	x	y
-2.32634787404	0.53473045192	0	-2.32634787404	0.534730425192
		$1/3$	-2.09064561365	0.225988241143
		1	-1.61924109285	-3.65816279362
1.0	0.0	0	1.0	0.0
		$1/3$	0.235702260396	0.691257815951
		1	0.707106781187	-3.19289321881

3 Attenuation

Associated external model: `attenuate.py`

Attenuation evaluation for quantity of interest u with input parameters $Y = [y_1, \ldots, y_N]$:

$$u(Y) = \prod_{n=1}^{N} e^{-y_n/N}. \tag{3}$$

This is the solution to the exit strength of a monodirectional, single-energy beam of neutral particles incident on a unit length material divided into N sections with independently-varying absorption cross sections. This test is useful for its analytic statistical moments as well as difficulty to represent exactly using polynomial representations.

3.1 Uniform

Let all y_n be uniformly distributed between 0 and 1. The first two statistical moments are:

3.1.1 mean

$$\begin{aligned}
\mathbb{E}[u(Y)] &= \int_0^1 dY \rho(Y) u(Y), \\
&= \int_0^1 dy_1 \cdots \int_0^1 dy_N \prod_{n=1}^{N} e^{-y_n/N}, \\
&= \left[\int_0^1 dy e^{-y/N}\right]^N, \\
&= \left[\left(-N e^{-y/N}\right)\Big|_0^1\right]^N, \\
&= \left[N\left(1 - e^{-1/N}\right)\right]^N.
\end{aligned} \tag{4}$$

3.1.2 variance

$$
\begin{aligned}
\mathbb{E}[u(Y)^2] &= \int_0^1 dY \rho(Y) u(Y), \\
&= \int_0^1 dy_1 \cdots \int_0^1 dy_N \frac{1}{1^N} \left(\prod_{n=1}^{N} e^{-y_n/N} \right)^2, \\
&= \left[\left(\int_0^1 dy \, e^{-2y/N} \right) \right]^N, \\
&= \left[\left(\frac{N}{2} e^{-2y/N} \right) \Big|_0^1 \right]^N, \qquad (5) \\
&= \left[\frac{N}{2} \left(1 - e^{-2/N} \right) \right]^N. \\
\mathrm{var}[u(Y)] &= \mathbb{E}[u(Y)^2] - \mathbb{E}[u(Y)]^2, \\
&= \left[\frac{N}{2} \left(1 - e^{-2/N} \right) \right]^N - \left[N \left(1 - e^{-1/N} \right) \right]^{2N}. \qquad (6)
\end{aligned}
$$

3.1.3 numeric values

Some numeric values for the mean and variance are listed below for several input cardinalities N.

N	mean	variance
2	0.61927248698470190	0.01607798775751018
4	0.61287838657652779	0.00787849640356994
6	0.61075635579491642	0.00520852933409887

3.2 Multivariate Normal

Let Y be N-dimensional, and have a multivariate normal distribution:

$$Y \sim N(\mu, \Sigma) \qquad (7)$$

with N-dimensional mean vector $\mu = [\mu_{y_1}, \mu_{y_2}, \ldots, \mu_{y_N}]$, and NXN covariance matrix:

$$\Sigma = [Cov[y_i, y_j]], i = 1, 2, \ldots, N; j = 1, 2, \ldots, N \qquad (8)$$

To be simplicity, we assume there are no correlations between the input parameters. Then, the covariance matrix can be written as:

$$\Sigma = \begin{pmatrix} \sigma_{y_1}^2 & 0 & \dots & 0 \\ 0 & \sigma_{y_2}^2 & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & \sigma_{y_N}^2 \end{pmatrix} \tag{9}$$

where $\sigma_{y_i}^2 = Cov[y_i, y_i]$, for $i = 1, 2, \dots, N$. Based on this assumption, the first two statistical moments are:

3.2.1 mean

$$\begin{aligned} \mathbb{E}[u(Y)] &= \int_{-\infty}^{\infty} dY \rho(Y) u(Y) \\ &= \int_{-\infty}^{\infty} dy_1 (1/\sqrt{2\pi\sigma_{y_1}} e^{-\frac{(y_1-\mu_{y_1})^2}{2\sigma_{y_1}^2}}) \cdots \int_{-\infty}^{\infty} dy_N (1/\sqrt{2\pi\sigma_{y_N}} e^{-\frac{(y_N-\mu_{y_N})^2}{2\sigma_{y_N}^2}}) \prod_{n=1}^{N} e^{-y_n/N} \\ &= \prod_{n=1}^{N} e^{\frac{\sigma_{y_i}^2}{2n^2} - \frac{\mu_{y_i}}{n}}. \end{aligned} \tag{10}$$

3.2.2 variance

$$\begin{aligned} \text{var}[u(Y)] = \mathbb{E}[(u(Y) - \mathbb{E}[u(Y)])^2] &= \int_{-\infty}^{\infty} dY \rho(Y) (u(Y) - \mathbb{E}[u(Y)])^2 \\ &= \int_{-\infty}^{\infty} dy_1 (1/\sqrt{2\pi\sigma_{y_1}} e^{-\frac{(y_1-\mu_{y_1})^2}{2\sigma_{y_1}^2}}) \\ &\cdots \int_{-\infty}^{\infty} dy_N (1/\sqrt{2\pi\sigma_{y_N}} e^{-\frac{(y_N-\mu_{y_N})^2}{2\sigma_{y_N}^2}}) (\prod_{n=1}^{N} e^{-y_n/N} - \mathbb{E}[u(Y)])^2 \\ &= \prod_{n=1}^{N} e^{\frac{2\sigma_{y_i}^2}{n^2} - \frac{2\mu_{y_i}}{n}}. \end{aligned} \tag{11}$$

3.2.3 numeric values

For example, for given mean $\mu = [0.5, -0.4, 0.3, -0.2, 0.1]$, and covariance

$$\Sigma = \begin{pmatrix} 0.64 & 0 & 0 & 0 & 0 \\ 0 & 0.49 & 0 & 0 & 0 \\ 0 & 0 & 0.09 & 0 & 0 \\ 0 & 0 & 0 & 0.16 & 0 \\ 0 & 0 & 0 & 0 & 0.25 \end{pmatrix} \tag{12}$$

The mean and variance can computed using previous equation, and the results are:

$$\mathbb{E}[u(Y)] = 0.97297197488624509 \tag{13}$$

$$\text{var} u(Y) = 0.063779804051749989 \tag{14}$$

3.3 Changing lower, upper bounds

A parametric study can be made by changing the lower and upper bounds of the material opacities.

The objective is to determine the effects on the exit strength u of a beam impinging on a unit-length material subdivided into two materials with opacities y_1, y_2. The range of values for these opacities varies from lower bound y_ℓ to higher bound y_h, and the bounds are always the same for both opacities.

We consider evaluating the lower and upper bounds on a grid, and determine the expected values for the opacity means and exit strength.

The analytic values for the exit strength expected value depends on the lower and upper bound as follows:

$$\bar{u}(y_1, y_2) = \int_{y_\ell}^{y_h} \int_{y_\ell}^{y_h} \left(\frac{1}{y_h - y_\ell} \right)^2 e^{-(y_1+y_2)/2} dy_1 dy_2, \tag{15}$$

$$= \frac{4e^{-y_h - y_\ell} \left(e^{y_h/2} - e^{y_\ell/2} \right)^2}{(y_h - y_\ell)^2}. \tag{16}$$

Numerically, the following grid points result in the following expected values:

y_ℓ	y_h	$\bar{y}_1 = \bar{y}_2$	$\bar{u}$
0.00	0.50	0.250	0.782865
0.00	0.75	0.375	0.695381
0.00	1.00	0.500	0.619272
0.25	0.50	0.375	0.688185
0.25	0.75	0.500	0.609696
0.25	1.00	0.625	0.541564
0.50	0.50	0.500	0.606531
0.50	0.75	0.625	0.535959
0.50	1.00	0.750	0.474832

4 Tensor Polynomial (First-Order)

Associated external model: `tensor_poly.py`

Tensor polynomial evaluation for quantity of interest u with input parameters $Y = [y_1, \ldots, y_N]$:

$$u(Y) = \prod_{n=1}^{N} y_n + 1. \tag{17}$$

This test is specifically useful for its analytic statistical moments. It is used as a benchmark in [1].

4.1 Uniform, (-1,1)

Let all y_n be uniformly distributed between -1 and 1. The first two statistical moments are:

4.1.1 mean

$$\begin{aligned}
\mathbb{E}[u(Y)] &= \int_{-1}^{1} dY \rho(Y) u(Y), \\
&= \int_{-1}^{1} dy_1 \cdots \int_{-1}^{1} dy_N \prod_{n=1}^{N} \frac{y_n+1}{2}, \\
&= \left[\int_{-1}^{1} dy \frac{y+1}{2} \right]^N, \\
&= \left[\frac{1}{2} \left(\frac{y^2}{2} + y \right) \Big|_{-1}^{1} \right]^N, \\
&= \left[\frac{2}{2} \right]^N, \\
&= 1.
\end{aligned} \tag{18}$$

4.1.2 variance

$$
\begin{aligned}
\mathbb{E}[u(Y)^2] &= \int_{-1}^{1} dY \rho(Y) u(Y), \\
&= \int_{-1}^{1} dy_1 \cdots \int_{-1}^{1} dy_N \frac{1}{2^N} \left(\prod_{n=1}^{N} y_n + 1 \right)^2, \\
&= \left[\frac{1}{2} \left(\int_{-1}^{1} dy\, y^2 + 2y + 1 \right) \right]^N, \qquad (19) \\
&= \left[\frac{1}{2} \left(\frac{y^3}{3} + y^2 + y \right) \Big|_{-1}^{1} \right]^N, \\
&= \left[\frac{1}{3} + 1 \right]^N, \\
&= \left(\frac{4}{3} \right)^N. \\
\text{var}[u(Y)] &= \mathbb{E}[u(Y)^2] - \mathbb{E}[u(Y)]^2, \\
&= \left(\frac{4}{3} \right)^N - 1. \qquad (20)
\end{aligned}
$$

4.1.3 numeric values

Some numeric values for the mean and variance are listed below for several input cardinalities N.

N	mean	variance
2	1.0	0.77777777777
4	1.0	2.16049382716
6	1.0	4.61865569273

4.2 Uniform, (0,1)

Let all y_n be uniformly distributed between 0 and 1. The first two statistical moments are:

4.2.1 mean

$$
\begin{aligned}
\mathbb{E}[u(Y)] &= \int_0^1 dY \rho(Y) u(Y), && (21)\\
&= \int_0^1 dy_1 \cdots \int_0^1 dy_N \prod_{n=1}^{N} y_n + 1, && (22)\\
&= \left[\int_0^1 dy y + 1 \right]^N, && (23)\\
&= \left[\left(\frac{y^2}{2} + y \right) \Big|_0^1 \right]^N, && (24)\\
&= \left[\frac{3}{2} \right]^N. && (25)
\end{aligned}
$$

4.2.2 variance

$$
\begin{aligned}
\mathbb{E}[u(Y)^2] &= \int_0^1 dY \rho(Y) u(Y), && (26)\\
&= \int_0^1 dy_1 \cdots \int_0^1 dy_N \left(\prod_{n=1}^{N} y_n + 1 \right)^2, && (27)\\
&= \left[\left(\int_0^1 dy\, y^2 + 2y + 1 \right) \right]^N, && (28)\\
&= \left[\left(\frac{y^3}{3} + y^2 + y \right) \Big|_0^1 \right]^N, && (29)\\
&= \left(\frac{7}{3} \right)^N. && (30)\\
\text{var}[u(Y)] &= \mathbb{E}[u(Y)^2] - \mathbb{E}[u(Y)]^2, && (31)\\
&= \left(\frac{7}{3} \right)^N - \left(\frac{3}{2} \right)^{2N}. && (32)
\end{aligned}
$$

4.2.3 numeric values

Some numeric values for the mean and variance are listed below for several input cardinalities N.

N	mean	variance
2	2.25	0.38194444444
4	5.0625	4.01306905864
6	11.390625	31.6377499009

4.3 Multivariate Normal

Let Y be N-dimensional, and have a multivariate normal distribution:

$$Y \sim N(\mu, \Sigma) \tag{33}$$

with N-dimensional mean vector $\mu = [\mu_{y_1}, \mu_{y_2}, \ldots, \mu_{y_N}]$, and NXN covariance matrix:

$$\Sigma = [Cov[y_i, y_j]], i = 1, 2, \ldots, N; j = 1, 2, \ldots, N \tag{34}$$

To be simplicity, we assume there are no correlations between the input parameters. Then, the covariance matrix can be written as:

$$\Sigma = \begin{pmatrix} \sigma_{y_1}^2 & 0 & \ldots & 0 \\ 0 & \sigma_{y_2}^2 & \ldots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \ldots & \sigma_{y_N}^2 \end{pmatrix} \tag{35}$$

where $\sigma_{y_i}^2 = Cov[y_i, y_i]$, for $i = 1, 2, \ldots, N$. Based on this assumption, the first two statistical moments are:

4.3.1 mean

$$\begin{aligned} \mathbb{E}[u(Y)] &= \int_{-\infty}^{\infty} dY \rho(Y) u(Y), \\ &= \int_{-\infty}^{\infty} dy_1 (1/\sqrt{2\pi\sigma_{y_1}} e^{-\frac{(y_1-\mu_{y_1})^2}{2\sigma_{y_1}^2}}) \cdots \int_{-\infty}^{\infty} dy_N (1/\sqrt{2\pi\sigma_{y_N}} e^{-\frac{(y_N-\mu_{y_N})^2}{2\sigma_{y_N}^2}}) \prod_{n=1}^{N} (y_n + 1), \\ &= \prod_{n=1}^{5} (\mu_{y_n} + 1). \end{aligned} \tag{36}$$

4.3.2 variance

$$
\begin{aligned}
\text{var}[u(Y)] = \mathbb{E}[(u(Y) - \mathbb{E}[u(Y)])^2] &= \int_{-\infty}^{\infty} dY \rho(Y)(u(Y) - \mathbb{E}[u(Y)])^2, \\
&= \int_{-\infty}^{\infty} dy_1 (1/\sqrt{2\pi\sigma_{y_1}} e^{-\frac{(y_1-\mu_{y_1})^2}{2\sigma_{y_1}^2}}), \\
&\cdots \int_{-\infty}^{\infty} dy_N (1/\sqrt{2\pi\sigma_{y_N}} e^{-\frac{(y_N-\mu_{y_N})^2}{2\sigma_{y_N}^2}})(\prod_{n=1}^{N}(y_n + 1 - \mathbb{E}[u(Y)])^2, \\
&= \prod_{n=1}^{5}[(1+\mu_{y_n})^2 + \sigma_{y_n}^2] - [\prod_{n=1}^{5}(\mu_{y_n}+1)]^2.
\end{aligned}
\tag{37}
$$

4.3.3 numeric values

For example, for given mean $\mu = [0.5, -0.4, 0.3, -0.2, 0.1]$, and covariance

$$
\Sigma = \begin{pmatrix} 0.64 & 0 & 0 & 0 & 0 \\ 0 & 0.49 & 0 & 0 & 0 \\ 0 & 0 & 0.09 & 0 & 0 \\ 0 & 0 & 0 & 0.16 & 0 \\ 0 & 0 & 0 & 0 & 0.25 \end{pmatrix} \tag{38}
$$

The mean and variance can computed using previous equation, and the results are:

$$
\mathbb{E}[u(Y)] = 1.0296 \tag{39}
$$

$$
\text{var}[u(Y)] = 4.047085600000002 \tag{40}
$$

5 Stochastic Collocation with Gamma Distribution

Associated external model: `poly_scgpc_gamma.py`

Recall that the *Gamma* distribution has the probability density function

$$f(x) = \frac{x^{\alpha-1}e^{-x/\beta}}{\beta^{\alpha}\Gamma(\alpha)}, \alpha > 0, \beta > 0 \tag{41}$$

The following two polynomials are used to compute the analytic statistical moments: *Gamma* distribution:

$$u_1(x, y) = x + y \tag{42}$$

$$u_2(x, y) = x^2 + y^2 \tag{43}$$

where x and y are two mutually independent *Gamma* variates, i.e.

$$x \sim \Gamma(\alpha_1, \beta_1)$$
$$y \sim \Gamma(\alpha_2, \beta_2)$$

5.1 Mean and Variance

The first two statistical moments of $u_1(x, y)$ and $u_2 x, y$ are:

$$\begin{aligned}
\mathbb{E}[u_1(x, y)] &= \int_0^{\infty} dxdyP(x, y)\, u_1(x, y)\,, \\
&= \int_0^{\infty} dxdy\Gamma(\alpha_1, \beta_1)\,\Gamma(\alpha_2, \beta_2)\, u_1(x, y)\,, \\
&= \frac{\alpha_1}{\beta_1} + \frac{\alpha_2}{\beta_2}
\end{aligned} \tag{44}$$

$$\begin{aligned}
\mathbb{E}[u_2(x, y)] &= \int_0^{\infty} dxdyP(x, y)\, u_2(x, y)\,, \\
&= \int_0^{\infty} dxdy\Gamma(\alpha_1, \beta_1)\,\Gamma(\alpha_2, \beta_2)\, u_2(x, y)\,, \\
&= \frac{(\alpha_1 + 1)\,\alpha_1}{\beta_1^2} + \frac{(\alpha_2 + 1)\,\alpha_2}{\beta_2^2}
\end{aligned} \tag{45}$$

$$\begin{aligned}
\text{var}[u_1(x, y)] &= \int_0^{\infty} dxdyP(x, y)\,[u_1(x, y) - \mathbb{E}[u_1(x, y)]]^2\,, \\
&= \frac{\alpha_1}{\beta_1^2} + \frac{\alpha_2}{\beta_2^2}
\end{aligned} \tag{46}$$

$$\text{var}[u_2(x,y)] = \int_0^{\infty} dxdyP\left(x,y\right)\left[u_2\left(x,y\right) - \mathbb{E}[u_2(x,y)]\right]^2 ,$$
$$= \frac{\left(4\alpha_1 + 6.0\right)\left(\alpha_1 + 1\right)\alpha_1}{\beta_1^4} + \frac{\left(4\alpha_2 + 6.0\right)\left(\alpha_2 + 1\right)\alpha_2}{\beta_2^4} \tag{47}$$

5.2 numeric values

Some numeric values for the mean and variance are listed below for given distributions:

$$x \sim \Gamma\left(11, 5\right)$$
$$y \sim \Gamma\left(2, 0.8\right)$$

$Function$	mean	variance
u_1	4.7	3.565
u_2	14.655	215.638125

6 Global Sobol Sensitivity: Sudret

Associated external model: `sudret_sobol_poly.py`

This model provides analytic Sobol sensitivities for a flexible number of input parameters. It is taken from [2] and has the following form:

$$u(Y) = \frac{1}{2^N} \prod_{n=1}^{N} \left(3y_n^2 + 1\right) . \tag{48}$$

The variables y_n are distributed uniformly on [0,1]. For three input variables ($N = 3$), the Sobol sensitivities are as follows, to 12 digits of accuracy:

$$S_1 = S_2 = S_3 = \frac{25}{91} \quad (0.2747), \tag{49}$$

$$S_{1,2} = S_{1,3} = S_{2,3} = \frac{5}{91} \quad (0.0549), \tag{50}$$

$$S_{1,2,3} = \frac{1}{91} \quad (0.0110). \tag{51}$$

The mean is 1.0 and the variance is 0.728.

6.1 Second-Order ANOVA of Second-Order Cut-HDMR Expansion of Sudret

One particular analytic tests involves calculating Sobol sensitivities for the second-order cut-HDMR expansion of the Sudret. We use three variables and equate $u(Y) = f(x, y, z)$. The reference cut point is $(\bar{x}, \bar{y}, \bar{z}) = (\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$.

The first step is to construct the second-order cut-HDMR expansion T,

$$f(x, y, z) \approx T[f](x, y, z) = t_r + t_x + t_y + t_z + t_{xy} + t_{xz} + t_{yz}, \tag{52}$$

$$t_r \equiv f(\bar{x}, \bar{y}, \bar{z}), \tag{53}$$

$$t_x \equiv f(x, \bar{y}, \bar{z}) - t_r, \tag{54}$$

$$t_{xy} \equiv f(x, y, \bar{z}) - t_x - t_y - t_r. \tag{55}$$

Symmetry between x, y, z provides similar expressions for the remaining terms. The cut-plane evaluations are

$$f_0 = t_r \equiv f(\bar{x}, \bar{y}, \bar{z}) = \frac{343}{512}, \tag{56}$$

$$f_x \equiv f(x, \bar{y}, \bar{z}) = \frac{49}{128}(3x^2 + 1), \tag{57}$$

$$f_{xy} \equiv f(x, y, \bar{z}) = \frac{7}{32}(3x^2 + 1)(3y^2 + 1), \tag{58}$$

and similar for the remaining terms. Expanding the cut-HDMR expression,

$$\begin{aligned} T[f](x, y, z) = t_r + (f_x - t_r) + (f_y - t_r) + (f_y - t_r) + \\ [f_{xy} - (f_x - t_r) - (f_y - t_r) - t_r] + \\ [f_{xz} - (f_x - t_r) - (f_z - t_r) - t_r] + \\ [f_{yz} - (f_y - t_r) - (f_z - t_r) - t_r], \end{aligned} \tag{59}$$

and collecting terms

$$T[f](x, y, z) = t_r - f_x - f_y - f_z + f_{xy} + f_{xz} + f_{yz}. \tag{60}$$

The ANOVA terms are recovered by integration of the cut-HDMR expansion. The ANOVA expansion H is similar in appearance to the cut-HDMR but uses different definitions; in fact, cut-HDMR is a coarse approximation of the ANOVA expansion. Here we use ANOVA to approximate the cut-HDMR expansion, instead of the original model.

$$H[T](x, y, z) = h_0 + h_x + h_y + h_z + h_{xy} + h_{xz} + h_{yz}, \tag{61}$$

$$h_0 \equiv \int_0^1 \int_0^1 \int_0^1 T[f](x, y, z)\, dx\, dy\, dz, \tag{62}$$

$$h_x \equiv \int_0^1 \int_0^1 T[f](x, y, z)\, dy\, dz - h_0, \tag{63}$$

$$h_{xy} \equiv \int_0^1 T[f](x, y, z)\, dz - h_x - h_y - h_0, \tag{64}$$

and similarly for the remaining terms. We evaluate the necessary integrals in the expansion.

$$\begin{aligned} \int_0^1 \int_0^1 \int_0^1 T[f](x, y, z)\, dxdydz &= \int_0^1 \int_0^1 \int_0^1 t_r - f_x - f_y - f_z + f_{xy} + f_{xz} + f_{yz}\, dxdydz, \\ &= \frac{343}{512} - 3\left(\frac{49}{64}\right) + 3\left(\frac{7}{8}\right), \\ &= \frac{511}{512}. \end{aligned}$$

$$h_0 = \int_0^1 \int_0^1 \int_0^1 T[f](x, y, z)\, dxdydz = \frac{511}{512}. \tag{65}$$

$$\begin{aligned} \int_0^1 \int_0^1 T[f](x, y, z)\, dxdy &= \int_0^1 \int_0^1 t_r - f_x - f_y - f_z + f_{xy} + f_{xz} + f_{yz}\, dxdy, \\ &= \frac{259}{512} + \frac{189}{128}z^2. \end{aligned}$$

$$h_z = \int_0^1 \int_0^1 T[f](x,y,z)\, dxdy - h_0 = \frac{259}{512} + \frac{189}{128}z^2 - \frac{511}{512} = -\frac{63}{128} + \frac{189}{128}z^2. \tag{66}$$

$$\begin{aligned}\int_0^1 T[f](x,y,z)\, dx &= \int_0^1 t_r - f_x - f_y - f_z + f_{xy} + f_{xz} + f_{yz}\, dx, \\ &= \frac{119}{512} + \frac{105}{128}(y^2+z^2) + \frac{63}{32}y^2z^2,\end{aligned}$$

$$\begin{aligned}h_{yz} &= \int_0^1 T[f](x,y,z)\, dx - h_y - h_z - h_0, \\ &= \frac{119}{512} + \frac{105}{128}(y^2+z^2) + \frac{63}{32}y^2z^2 - \\ &= \frac{7}{32} - \frac{21}{32}(y^2+z^2) + \frac{63}{32}y^2z^2.\end{aligned} \tag{67}$$

The other terms are obtained similarly, and are symmetric. In summary,

$$h_0 = \frac{511}{512}, \tag{68}$$

$$h_x = -\frac{63}{128} + \frac{189}{128}x^2, \tag{69}$$

$$h_y = -\frac{63}{128} + \frac{189}{128}y^2, \tag{70}$$

$$h_z = -\frac{63}{128} + \frac{189}{128}z^2, \tag{71}$$

$$h_{xy} = \frac{7}{32} - \frac{21}{32}(x^2+y^2) + \frac{63}{32}x^2y^2, \tag{72}$$

$$h_{xz} = \frac{7}{32} - \frac{21}{32}(x^2+z^2) + \frac{63}{32}x^2z^2, \tag{73}$$

$$h_{yz} = \frac{7}{32} - \frac{21}{32}(y^2+z^2) + \frac{63}{32}y^2z^2. \tag{74}$$

It can be shown that the expectation value of any ANOVA expansion term is zero, with the exception of the first term h_0. Additionally, each term is orthogonal to each other term. The second moment can thus be calculated as

$$\begin{aligned}\langle H[T](x,y,z)^2 \rangle &\equiv \int_0^1 \int_0^1 \int_0^1 (h_0 + h_x + h_y + h_z + h_{xy} + h_{xz} + h_{yz})^2\, dxdydz, \\ &= h_0^2 + \int_0^1 \int_0^1 \int_0^1 h_x^2 + h_y^2 + h_z^2 + h_{xy}^2 + h_{xz}^2 + h_{yz}^2\, dxdydz.\end{aligned} \tag{75}$$

To obtain the variance σ^2_{tot}, we subtract the square of the mean,

$$\sigma^2_{\text{tot}} = \int_0^1 \int_0^1 \int_0^1 h_x^2 + h_y^2 + h_z^2 + h_{xy}^2 + h_{xz}^2 + h_{yz}^2\, dxdydz. \tag{76}$$

The partial variance σ_k^2 of any subset k is the integral of the square of that ANOVA term.

$$\sigma_x^2 = \sigma_y^2 = \sigma_z^2 = \frac{3969}{20480} \approx 0.19379883, \tag{77}$$

$$\sigma_{xy}^2 = \sigma_{xz}^2 = \sigma_{yz}^2 = \frac{49}{1600} = 0.030625. \tag{78}$$

The total variance is a sum of the partial variances,

$$\sigma_{\text{tot}}^2 = 3\left(\frac{3969}{20480}\right) + 3\left(\frac{49}{1600}\right) = \frac{68943}{102400} \approx 0.67327. \tag{79}$$

The Sobol indices are the ratio of the partial variance to the total,

$$\mathcal{S}_x = \mathcal{S}_y = \mathcal{S}_z = \frac{135}{469} \approx 0.287846482, \tag{80}$$

$$\mathcal{S}_{xy} = \mathcal{S}_{xz} = \mathcal{S}_{yz} = \frac{64}{1407} \approx 0.045486851. \tag{81}$$

7 Global Sobol Sensitivity: Ishigami

Associated external model: `ishigami.py`

This model has interesting properties for its sensitivity indices, in that y_3 has zero impact alone but a nonzero impact when coupled with y_1. Additionally, the sinusoidal expression is not trivially represented by polynomial expansion. It is listed in [3] and has the following form:

$$u(Y) = \sin(y_1) + a\sin^2(y_2) + by_3^4\sin(y_1), \tag{82}$$

where in this case $a = 7$ and $b = 0.1$, and all y_n are uniformly distributed on $[-\pi, \pi]$.

The variance and partial variances are as follows:

$$D_{\text{tot}} = \frac{a^2}{8} + \frac{b\pi^4}{5} + \frac{b^2\pi^8}{18} + \frac{1}{2}, \tag{83}$$

$$D_1 = \frac{b\pi^4}{5} + \frac{b^2\pi^8}{50} + \frac{1}{2}, \tag{84}$$

$$D_2 = \frac{a^2}{8}, \tag{85}$$

$$D_3 = 0, \tag{86}$$

$$D_{1,2} = 0, \tag{87}$$

$$D_{2,3} = 0, \tag{88}$$

$$D_{1,3} = \frac{8b^2\pi^8}{225}, \tag{89}$$

$$D_{1,2,3} = 0. \tag{90}$$

The corresponding variance values and Sobol sensitivities are listed in Table 1.

Variable	Partial Variance	Sobol Index	Sobol Total Index
(total)	13.8446	1	-
y_1	4.34589	0.3138	0.5574
y_2	6.125	0.4424	0.4424
y_3	0	0	0.2436
y_1, y_2	0	0	-
y_1, y_3	3.3737	0.2436	-
y_2, y_3	0	0	-
y_1, y_2, y_3	0	0	-

Table 1. Ishigami sensitivities and variances

8 Sobol G-Function

Associated external model: `gFunction.py`

This function developed by Sobol has the benefit of tuning factors a_n that allow the importance of any particular term to be increased or decreased. Because of the absolute value, this function is quite challenging for polynomial expansion. Documentation can be found in [4]. The function is represented by

$$u(Y) = \prod_{n=1}^{N} \frac{|4y_n - 2| + a_n}{1 + a_n}, \tag{91}$$

where y_n are distributed uniformly on [0,1] and a_n are non-negative. a_n are generally integers, and smaller values lead to greater impact of corresponding y_n. As in [2] we use $N = 8$ with $a = [1, 2, 5, 10, 20, 50, 100, 500]$. The partial variances are given by

$$D_n = \frac{1}{3(1 + a_n)^2}, \tag{92}$$

$$D_{\text{tot}} = \prod_{n=1}^{N} (D_n + 1) - 1. \tag{93}$$

Analytic values for Sobol sensitivities are given in Table 2.

Variable	Sobol sensitivity	Sobol total sensitivity
y_1	0.6037	0.6342
y_2	0.2683	0.2945
y_3	0.0671	0.0756
y_4	0.0200	0.0227
y_5	0.0055	0.0062
y_6	0.0009	0.0011
y_7	0.0002	0.0003
y_8	0.0000	0.0000

Table 2. G-Function sensitivities and variances

9 Risk Importance Measures

Associated test: `tests/framework/PostProcessors/InterfacedPostProcessor/test-riskMeasuresDiscreteMultipleIE.xml` Risk Importance Measures (RIMs) are originally defined for each basic event in a Event-Tree/Fault-Tree analysis. In a simulation based environment similar calculations can employed for boolean models.

For each component i and for each IE the following quantities are calculated:

- R^0 = probability of system failure
- R^i_+ = probability of system failure given component i has failed
- R^i_- = probability of system failure given component i is prefectly reliable

For each component i, four RIMs indexes can be computed:

- $RAW^i = R^i_-/R^0$
- $RAW^i = R^0/R^i_+$
- $B^i = R^i_- R^i_+$
- $FV^i = (R^0 - R^i_-)/R^0$

In the asscoiated test, a system composed by four components (i.e., A, B, C and D) is analyzed for 2 Initiating Events (IEs), IE1 and IE2. Data associated for each IE is as follows:

- IE1 (probability $p1 = 0.01$); 1 single MCS, $MCS1 = A + BC$
- IE2 (probability $p1 = 0.02$); 1 single MCS, $MCS2 = BCD$

In the associated test, the following probabilities are provided:

- $p_A = 0.01$
- $p_B = 0.05$
- $p_C = 0.1$
- $p_D = 0.02$

Table 3. IE1: symbolic expressions of R^0, R^i_+ and R^i_-

	$R0$	R^i_+	R^i_-
A	A+BC	[]	BC
B	A+BC	A+C	A
C	A+BC	A+B	A
D	A+BC	A+BC	A+BC

Table 4. IE1: numerical value of R^0, R^i_+ and R^i_-

	$R0$	R^i_+	R^i_-
A	0.01495	1.0	0.005
B	0.01495	0.109	0.01
C	0.01495	0.0595	0.01
D	0.01495	0.01495	0.01495

Table 5. IE2: symbolic expressions of R^0, R^i_+ and R^i_-

	$R0$	R^i_+	R^i_-
A	BCD	BCD	BCD
B	BCD	CD	-
C	BCD	BD	-
D	BCD	BC	BCD

Table 6. IE2: numerical value of R^0, R^i_+ and R^i_-

	$R0$	R^i_+	R^i_-
A	0.0001	0.0001	0.0001
B	0.0001	0.002	0.0
C	0.0001	0.001	0.0
D	0.0001	0.005	0.0

For each IE, the symbolic expressions and the numerical expressions of R^0, R^i_+ and R^i_- are calculated (see Tables 3, 4, 5 and 6).

Given the values provided above it is possible to linearly weight them with the probability associated to each IE (see Table 7).

Table 7. IE1+IE2: numerical value for R^0, R^i_+ and R^i_-

	$R0$	R^i_+	R^i_-
A	0.0001515	0.010002	0.000052
B	0.0001515	0.00113	0.0001
C	0.0001515	0.000615	0.0001
D	0.0001515	0.0002495	0.0001495

Then, it is possible to obtain the values of each of the 4 RIMs for eah component:

Table 8. IE1+IE2: numerical value for R^0, R^i_+ and R^i_-

	RAW	RRW	FV	B
A	66.01980198	2.913461538	0.656765677	0.00995
B	7.458745875	1.515	0.339933993	0.00103
C	4.059405941	1.515	0.339933993	0.000515
D	1.646864686	1.013377926	0.01320132	0.0001

10 Parabolas

Associated external model: `parabolas.py`

This model is a simple N-dimensional parabolic response $u(Y)$,

$$u(Y) = \sum_{n=1}^{N} -y_n^2, \tag{94}$$

where the uncertain inputs are $Y = (y_1, \cdots, y_N)$ and can be defined arbitrarily. For optimization searches, it is possible to obtain a maximum in the interior of the input by assuring the range of each input variable include 0. In this case, the maximum point will be 0^N.

11 Fourier

Some signal processing tests make use of Fourier-based signals for analytic tests.

In constructing a Fourier signal, we use the formulation

$$f(t) = \sum_k \sin \frac{2\pi}{k \in \Lambda} t + \cos \frac{2\pi}{k} t, \qquad \Lambda \in \mathbb{R}^N, \tag{95}$$

where the choice of periods Λ is any arbitrary set of real numbers and can have any dimensionality.

If the resulting signal is treated by a fast fourier transform, it should show peaks at the frequencies corresponding to the selected periods, where frequencies are simply the inverse of the periods.

12 Optimization Functions

The functions in this section are models with analytic optimal points.

12.1 General

12.1.1 Beale's Function

Beale's function has a two-dimensional input space and a single global/local minimum. See `https://en.wikipedia.org/wiki/Test_functions_for_optimization`.

- Function: $f(x, y) = (1.5 - x + xy)^2 + (2.25 - x + xy^2)^2 + (2.625 - x + xy^3)^2$
- Domain: $-4.5 \leq x, y \leq 4.5$
- Global Minimum: $f(3, 0.5) = 0$

12.1.2 Rosenbrock Function

The Rosenbrock function can take a varying number of inputs. For up to three inputs, a single global minimum exists. For four to seven inputs, there is one local minimum and one global maximum. See `https://en.wikipedia.org/wiki/Rosenbrock_function`.

- Function: $f(\boldsymbol{x}) = \sum_{i=1}^{n-1} \left[100 \left(x_{i+1} - x_i^2\right)^2 + (x_i - 1)^2)\right]$
- Domain: $-\infty \leq x_i \leq \infty \quad \forall \quad 1 \leq i \leq n$
- Global Minimum: $f(1, 1, \cdots, 1, 1) = 0$
- Local minimum ($n \geq 4$): near $f(-1, 1, \cdots, 1)$

12.1.3 Goldstein-Price Function

The Goldstein-Price function is a two-dimensional input function with a single global minimum. See `https://en.wikipedia.org/wiki/Test_functions_for_optimization`.

- Function:

$$f(x,y) = \left[1 + (x+y+1)^2 \left(19 - 14x + 3x^2 - 14y + 6xy + 3y^2\right)\right] \cdot \left[30 + (2x-3y)^2(18 - 32x + 12x^2 + 48y - 36xy + 27y^2)\right] \quad (96)$$

- Domain: $-2 \leq x, y \leq 2$
- Global Minimum: $f(0, -1) = 3$

12.1.4 McCormick Function

The McCormick function is a two-dimensional input function with a single global minimum. See `https://en.wikipedia.org/wiki/Test_functions_for_optimization`.

- Function: $f(x,y) = \sin(x+y) + (x-y)^2 - 1.5x + 2.5y + 1$
- Domain: $-1.5 \leq x \leq 4$, $-3 \leq y \leq 4$
- Global Minimum: $f(-0.54719, -1.54719) = -1.9133$

12.1.5 2D Canyon

The two-dimensional canyon offers a low region surrounded by higher walls.

- Function: $f(x,y) = xy\cos(x+y)$
- Domain: $0 \leq x, y \leq \pi$
- Global Minimum: $f(1.8218, 1.8218) = -2.90946$

12.1.6 Time-Parabola

This model features the sum of a parabola in both x and y; however, the parabola in y moves in time and has a reduced magnitude as time increases. As such, the minimum is always found at $x = 0$ and at $(t - y) = 0$, with y values at low t being more impactful than at later t, and x as impactful as $y(t = 0)$.

- Function: $f(x,y,t) = x^2 + \sum_t (t-y)^2 \exp -t$
- Domain: $-10 \leq x, y, t \leq 10$
- Global Minimum: $f(0, y = t, t) = 0$

12.2 Constrained

12.2.1 Mishra's Bird Function

The Mishra bird function offers a constrained problem with multiple peaks, local minima, and one steep global minimum. See https://en.wikipedia.org/wiki/Test_functions_for_optimization.

- Function: $f(x, y) = \sin(y) \exp[1 - \cos(x)]^2 + \cos(x) \exp[1 - \sin(y)]^2 + (x - y)^2$
- Constraint: $(x + 5)^2 + (y + 5)^2 < 25$
- Domain: $-10 \leq x \leq 0$, $-6.5 \leq y \leq 0$
- Global Minimum: $f(-3.1302468, -1.5821422) = -106.7645367$

13 Processor Load

Associated external model: `stress.py`

The entire purpose of this model is to keep a processor at 100 percent utilization for a specified interval. It can be coupled with other models via an ensemble model to assure a calculation takes at least a certain period of time.

The input to this model is `interval`, which determines the number of seconds at which the model should run. The output is `done`, which always evaluates to 1.0.

Appendices

A Document Version Information

c493b48a9b9be1d4ed62895040407eb1781056f0 Congjian Wang Thu, 2 May 2019 12:35:07 -0600

References

[1] D. Ayres and M. D. Eaton, "Uncertainty quantification in nuclear criticality modelling using a high dimensional model representation," *Annals of Nuclear Energy*, vol. 80, pp. 379–402, May 2015.

[2] B. Sudret, "Global sensitivity analysis using polynomial chaos expansions," *Reliability Engineering and System Safety*, pp. 964–979, April 2007.

[3] A. Saltelli, K. Chan, E. Scott, and editors, *Sensitivity analysis*. New York: Wiley, 2000.

[4] I. Sobol, "Theorems and examples on high dimensional model representation," *Reliability Engineering and System Safety*, no. 79, pp. 187–193, 2003.

Idaho National Laboratory