Copulas for Uncertainty Analysis

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Jun 21st, 2010

Outline

- GUM
  - Refractive index
  - Shortcomings

- GUM SUPPLEMENT 1
  - Change-of-Variables Formula
  - Monte Carlo Method

- COPULAS
  - Definition & Illustrations
  - GUM Example H.2

Refractive Index

- Apex angle $\alpha$, refractive index $n$, immersed in medium with refractive index $m$

- Light enters prism at angle $\phi$, traverses prism’s body, and exits at angle $\psi$

- As prism rotates about light’s entrance point, $\delta = 2(\phi + \psi - \alpha)$ decreases, reaches minimum $\delta_M$, then increases

$$n = m \frac{\sin((\alpha + \delta_M)/2)}{\sin(\alpha/2)}$$

Refractive Index — Partial Derivatives

$$\dot{f}_m(m, \phi, \psi, \alpha) = \frac{\sin(\phi + \psi - \alpha/2)}{\sin(\alpha/2)}$$

$$\dot{f}_\phi(m, \phi, \psi, \alpha) = m \frac{\cos(\phi + \psi - \alpha/2)}{\sin(\alpha/2)}$$

$$\dot{f}_\psi(m, \phi, \psi, \alpha) = m \frac{\cos(\phi + \psi - \alpha/2)}{\sin(\alpha/2)}$$

$$\dot{f}_\alpha(m, \phi, \psi, \alpha) = -\frac{m}{2} \left[ \frac{\cos(\phi + \psi - \frac{\alpha}{2})}{\sin(\frac{\alpha}{2})} + \frac{\sin(\phi + \psi - \frac{\alpha}{2})}{\sin(\frac{\alpha}{2})\tan(\frac{\alpha}{2})} \right]$$
Streamlining Computation

- Computation of standard uncertainty using GUM’s Taylor approximation is tedious and error-prone, especially when measurement equation is non-linear or involves special functions.
- Employ software capable of computing derivatives:
  - Analytically (for example, Maple)
  - Numerically (for example, R)
    - R is freely available, and its source code is open: http://www.r-project.org/
    - metRology package (LGC / NIST)

GUM Approximation — Shortcomings

- If some first order partial derivatives of \( f \) are zero at values of input quantities, then GUM’s approximation may be faulty:
  - Radiant power \( W = \kappa \cos(A) \)
- GUM’s approximation may be poor when \( f \) is markedly non-linear in neighborhood of values of input quantities:
  - Need to study \( f \)’s curvature is extra burden
  - If curvature is appreciable and influential, need higher-order approximation
    - However, examples can be constructed where first-order approximation is better than second-order approximation — Wang & Iyer (2005)

GUM Approximation — More Shortcomings

- Expanded uncertainties and coverage intervals involve coverage factor whose value depends on generally unverifiable assumption that output quantity has Gaussian or Student’s \( t \) distribution
- Even when \( Y \sim t_\nu \), Welch-Satterthwaite formula often yields inappropriate value for \( \nu \)

Example (GUM H.1)

- \( l = l_S + d - l_S(1 - \delta \alpha \theta - \alpha_S \delta \theta) \)
- Welch-Satterthwaite formula yields \( \nu_{eff} = 16 \)
- GUM’s 99% coverage interval 17% longer than it needs to be

GUM Supplement 1 — Problem

- Given
  - Measurement equation \( Y = f(X_1, \ldots, X_n) \)
  - Joint probability distribution of \( X_1, \ldots, X_n \) (with density \( \varphi \))
- Determine \( Y \)’s probability distribution:
  - Derive \( Y \)’s density analytically
    — Change-of-variables formula
  - Sample \( Y \)’s distribution
Change of Variables Formula

- **Transformation** $\tau = (f, \tau_2, \ldots, \tau_n)$
  - One-to-one, continuously differentiable
  - Inverse has non-vanishing Jacobian

\[
Y = f(X_1, \ldots, X_n) \\
Z_2 = \tau_2(X_1, \ldots, X_n) \\
\ldots \\
Z_n = \tau_n(X_1, \ldots, X_n)
\]

- $Y$ has probability density $\psi$

\[
\psi(y) = \int_{z_2} \cdots \int_{z_n} \phi(\tau^{-1}(y, z_2, \ldots, z_n)) \\
\quad \quad |J_{\tau^{-1}}(y, z_2, \ldots, z_n)| \, dz_2 \ldots dz_n
\]

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**GUM Supplement 1 — Step 1**

**PROPAGATING DISTRIBUTIONS (MONTE CARLO)**

- **STEP 1:** Select probability distribution to describe state of knowledge about input quantities
  - If $X_1, \ldots, X_n$ can be regarded as independent random variables, then assign probability distributions to each one of them separately
  - Otherwise, assign multivariate distribution to all of them together **using a copula**
  - In either case, mean and standard deviation of each $X_j$'s distribution should be $x_j$ and $u(x_j)$

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**GUM Supplement 1 — Steps 2–4**

**PROPAGATING DISTRIBUTIONS (MONTE CARLO)**

- **STEP 2:** Choose suitably large number $K$ for size of sample to generate from probability distribution of output quantity
- **STEP 3:** Simulate $K$ vectors of values of input quantities, and compute $y_k = f(x_{k1}, \ldots, x_{kn})$ for $k = 1, \ldots, K$
- **STEP 4:** Assign to $u(y)$ (standard uncertainty of output quantity) the value of the standard deviation of $y_1, \ldots, y_K$

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**GUM Supplement 1 — Refractive Index (CI)**

- Use sample $\{y_1, \ldots, y_K\}$ to estimate probability density of prism's refractive index — most complete characterization of uncertainty
- Shaded region includes 95% of total area under curve: footprint on horizontal axis is a coverage interval for measurand with 95% confidence
### GUM Example H.2

#### INPUT QUANTITIES
- Amplitude $V$ of sinusoidally-alternating potential difference across electrical circuit’s terminals
- Amplitude $I$ of alternating current
- Phase-shift angle $\phi$ of alternating potential difference relative to alternating current
- $V$, $I$, and $\phi$ are correlated

#### OUTPUT QUANTITIES
- Resistance $R = \frac{V}{I}$ cos $\phi$
- Reactance $X = \frac{V}{I}$ sin $\phi$
- Impedance’s magnitude $Z = \frac{V}{I}$

### Problem & Solutions

#### PROBLEM
- Given probability distributions for input quantities, and correlations between them, how does one manufacture a joint probability distribution consistent with those margins and correlations?

#### SOLUTIONS
- There are infinitely many joint distributions that are consistent with given marginal distributions and correlations
- **Copulas** join univariate probability distributions into multivariate distributions and impose dependence structure

### Copulas are not Cupolas

Manufacturer mentioned solely to acknowledge image source, with no implied recommendation or endorsement by NIST that cupola portrayed is the best available for any particular purpose.
A copula is the cumulative distribution function of a multivariate distribution on the unit hypercube all of whose margins are uniform.

Clayton copula inducing Kendall’s $\tau = 0.6$.

Sklar’s (1959) Theorem

If $H$ is CDF of multivariate distribution whose margins have CDFs $F_1, \ldots, F_n$, then there exists copula $C$ such that

$$H(x_1,\ldots,x_n) = C(F_1(x_1),\ldots,F_n(x_n))$$

If $F_1, \ldots, F_n$ are continuous, then $C$ is unique.

$C(p_1,\ldots,p_n) = H(F_1^{-1}(p_1),\ldots,F_n^{-1}(p_n))$

Copula — Example: Definition

Example (Gaussian Copula on Beta Margins)

- $U \sim \text{BETA}(3, 5)$ has CDF $F$
- $V \sim \text{BETA}(4, 2)$ has CDF $G$
- $\rho = \text{cor}(U, V) = 0.7$
- Copula $C$ such that

$$C(p, q) = \Phi_p(F^{-1}(p), G^{-1}(q))$$

for $0 \leq p, q \leq 1$
Copula — Example: Joint Density

Influential Copulas

- Joint distributions with same Gaussian margins and same correlation

GUM Example H.2

OUTPUT QUANTITIES

- Resistance $R = \frac{V}{I} \cos \phi$
- Reactance $X = \frac{V}{I} \sin \phi$
- Impedance's magnitude $Z = \frac{V}{I}$

GUM Example H.2 — Data

<table>
<thead>
<tr>
<th>$V$ (V)</th>
<th>$I$ (mA)</th>
<th>$\phi$ (rad)</th>
</tr>
</thead>
<tbody>
<tr>
<td>5.007</td>
<td>19.663</td>
<td>1.0456</td>
</tr>
<tr>
<td>4.994</td>
<td>19.639</td>
<td>1.0438</td>
</tr>
<tr>
<td>5.005</td>
<td>19.640</td>
<td>1.0468</td>
</tr>
<tr>
<td>4.990</td>
<td>19.685</td>
<td>1.0428</td>
</tr>
<tr>
<td>4.999</td>
<td>19.678</td>
<td>1.0433</td>
</tr>
</tbody>
</table>
GUM Example H.2 — Evaluations

- Input quantity values estimated by averages $\bar{V}$, $\bar{I}$, and $\bar{\phi}$, of sets of five indications
- Uncertainties and correlations of input quantities assessed by Type A evaluations
  - $u(\bar{V}) = \text{SD}(5.007, 4.994, 5.005, 4.990, 4.999) / \sqrt{5}$
  - Similarly for $u(\bar{I})$ and $u(\bar{\phi})$
  - $\text{cor}(V, I)$, $\text{cor}(V, \phi)$, and $\text{cor}(I, \phi)$ estimated by correlations between paired sets of five indications

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GUM Example H.2 — GUM Supplement 1

CHALLENGES

- Quality of estimates of $u(V)$, $u(I)$, $u(\phi)$, $\text{cor}(V, I)$, $\text{cor}(V, \phi)$, and $\text{cor}(I, \phi)$ limited by very small number of indications they are based on
- Marginal distributions must be chosen for $V$, $I$ and $\phi$, and then linked using a copula that reproduces correlations between them

SOLUTION

- Employ Student $t_4$ distributions for
  \[
  \frac{\bar{V} - \mu_V}{u(\bar{V})}, \quad \frac{\bar{I} - \mu_I}{u(\bar{I})}, \quad \text{and} \quad \frac{\bar{\phi} - \mu_\phi}{u(\bar{\phi})}
  \]
- Tune Gaussian copula using correlation supplicant
- Apply copula
  - To sample correlation matrix
  - To use sampled correlation matrix in turn to sample output quantities
Correlation Supplicant

- Copula parameter $\theta$ determines dependence structure, in particular correlation matrix $\rho(\theta)$.

**Example**

- **STUDENT**: $\theta$ comprises $\nu$ and $\Sigma$.
- **CLAYTON**: $C(\rho, q) = (\rho^{-\theta} + q^{-\theta} - 1)^{-\frac{1}{\theta}}$, $\theta \geq -1$.

**Correlation Supplicant** selects $\theta$ that minimizes difference between $\rho$ and $\rho(\theta)$.

- Minimization with respect to $\theta$ done under constraint that $\rho(\theta)$ must be *bona fide* correlation matrix.

GUM Example H.2 — GUM Supplement 1

**RESULTS**

<table>
<thead>
<tr>
<th>GAUSSIAN COPULA WITH GAUSSIAN MARGINS</th>
<th>$R$ ($\Omega$)</th>
<th>$X$ ($\Omega$)</th>
<th>$Z$ ($\Omega$)</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>AVE</strong></td>
<td>127.7</td>
<td>219.8</td>
<td>254.3</td>
</tr>
<tr>
<td><strong>$u$</strong></td>
<td>0.0711</td>
<td>0.296</td>
<td>0.236</td>
</tr>
<tr>
<td><strong>$U_{99%}$</strong></td>
<td>0.18</td>
<td>0.76</td>
<td>0.61</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>GAUSSIAN COPULA WITH STUDENT MARGINS</th>
<th>$R$ ($\Omega$)</th>
<th>$X$ ($\Omega$)</th>
<th>$Z$ ($\Omega$)</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>AVE</strong></td>
<td>127.7</td>
<td>219.8</td>
<td>254.3</td>
</tr>
<tr>
<td><strong>$u$</strong></td>
<td>0.0828</td>
<td>0.289</td>
<td>0.232</td>
</tr>
<tr>
<td><strong>$U_{99%}$</strong></td>
<td>0.29</td>
<td>0.93</td>
<td>0.75</td>
</tr>
</tbody>
</table>

GUM Example H.2 — Results

GUM Example H.2 — Limitation

- All usual copulas fail to capture fact that joint distribution of $(R, X, Z)$ is degenerate:

  $$Z^2 = R^2 + X^2$$

- However, this is largely irrelevant in this case because relative standard uncertainties are very small — all less than $0.1\%$. 
Conclusions & Reference

- When input quantities are correlated, and their joint distribution is not determined otherwise, copula must be used to apply Monte Carlo Method of GUM Supplement 1

- Many different copulas can reproduce given correlations, yet lead to possibly very different uncertainty evaluations for output quantity