Remarks on uncertainty analysis in large-scale simulation models

Davit Stepanyan
*International Agricultural Trade and Development, Humboldt-Universität zu Berlin, Berlin, Germany. Corresponding author, email: davit.stepanyan@hu-berlin.de*

Khalid Siddig
*International Agricultural Trade and Development, Humboldt-Universität zu Berlin, Berlin, Germany and Khartoum University, the Sudan.*

Harald Grethe
*International Agricultural Trade and Development, Humboldt-Universität zu Berlin, Berlin, Germany.*

Georg Zimmermann
*Applied Mathematics and Statistics, Universität Hohenheim, Stuttgart, Germany.*

**Background**

Economic simulation models (ESMs) are often deterministic in nature making the results highly dependent on point estimates of key exogenous variables. One way to deal with uncertainty is the application of stochastics in ESMs. However, this step transforms the ESM into a problem of multiple numerical integrations. In order to evaluate those integrals, mostly two different approaches are applied: probabilistic formulae (e.g. Monte Carlo simulations) and efficient formulae (e.g. Gaussian Quadratures (GQ)).

In the first approach, the multiple integrals are evaluated as a probabilistic problem and investigated using statistical experiments (Metropolis & Ulam, 1949). However, such an approach requires large computational capacity as thousands of iterations are required for each stochastically treated exogenous variable (Haber, 1970), which makes this approach infeasible for large-scale ESMs. The Monte Carlo approach is an effective method and simple to apply. However, in order to reach reliable results via this approach, one needs a sufficient number of iterations (Arndt, 1996). The required sample size depends on many model characteristics, including the dimensionality of the model, different model asymmetries, etc. Haber (1970) suggests that the Monte Carlo sample size should range from 40,000 to 100,000.

For conducting sensitivity analysis GLOBIOM, FAPRI and Aglink-Cosimo models apply the Monte Carlo approach, however, using a relatively small and not validated sample size because of the limitations of the currently existing computational capacities. For example, in order to reach reliable (converged) results with the above-mentioned approach in a small partial equilibrium toy model\(^1\) representing 3 regions and 6 commodities 24,000 iterations and 24 hours of computational time were required (Fig. 1). Please note that in large-scale

\(^1\) A partial equilibrium toy model based on the structure of European Simulation Model (ESIM). (Grethe et al., 2012)
models the level of inaccuracies is significantly larger and consequently the number of points and the computational resources required are much bigger.

In contrast, efficient formulae require a minimal number of points (2n, where n is the number of the stochastically treated exogenous variables) to approximate the central moments of a joint probability distribution. GQ is an approach designed by Stroud (1957) and later adapted by Arndt (1996) to be applied in large-scale ESMs, in order to reduce the computational costs and receive reliable results. Currently, GQ is applied to GTAP (Channing Arndt, 1996) and ESIM (Artavia et al., 2015) models as a means of uncertainty analysis. The GQ-method allows for the random draw of order 3 GQs for symmetric distributions. The GQs will be exact if the integrand is a polynomial of order d ≤ 3 (Arndt, 1996). However, Arndt (1996) also accepts that in some cases the quality of approximation may deteriorate. For example, see Figure 2 which represents the coefficient of variation of EU potato prices received by solving the same partial equilibrium toy model as for the Monte Carlo approach using 18 different rotations of Stroud’s octahedron and the time required to solve each model. The results are compared with the ones obtained by 24,000 Monte Carlo runs. Although we observe that the results produced by the 18 different GQs are relatively close to the one produced by the 24,000 Monte Carlo runs there are still some obvious inaccuracies. As in the case of Monte Carlo approach, the inaccuracies caused by different rotations of the GQs grow larger in large-scale models.

![Figure 1](image_url)
Thus, in this paper, a new methodology to reduce the possible approximation error caused by different rotations of Stroud’s octahedron is presented. The experiment is performed in a large-scale recursive-dynamic CGE model addressing the Sudan.

**Methodology**

Stroud’s (1957) theorem of order 3 numerical integration formulas for symmetric regions states:

A necessary and sufficient condition that $2n$ points $v_1, \ldots, v_n, -v_1, \ldots, -v_n$ form an equally weighted numerical integration formula of degree 3 for a symmetrical region is that these points form the vertices of a $Q_n$ whose centroid coincides with the centroid of the region and lie on n-sphere of radius $r = \sqrt{nI_2 / I_0}$.  

Where $Q_n$ is the octahedron or any rotation of this region, $I_0$ is the n-volume of the region of integration and $I_2$ is the integral of the square of any variable over that region. Fig. 3 gives the geometrical depiction of the theorem:
The crucial condition of the above-mentioned formula is that the vertices of the octahedron fall inside the integration region (in this case the cube). However, Stroud was faced with the problem that whenever \( n > 3 \) (dimensionality) these points were falling outside of the region. Therefore, he suggested rotating the octahedron so that those points lie on the surface of the integration region. For that purpose, he suggested the following degree 3 equally weighted quadrature formulae for the \( n \)-cube with vertices \((\pm1, \pm1, \ldots, \pm1)\) (Stroud, 1957):

Let \( \Gamma_k \) denote the point \((\gamma_1, \gamma_2, \ldots, \gamma_n)\) where

\[
\gamma_{2r-1} = \sqrt{2} \frac{\cos \left(\frac{(2r-1)k\pi}{n}\right)}{3} \quad \gamma_{2r-1} = \sqrt{2} \frac{\sin \left(\frac{(2r-1)k\pi}{n}\right)}{3} \quad r=1,2,\ldots,\left[\frac{n}{2}\right],
\]

if \( n \) is odd \( \gamma_n = (-1)^k \sqrt{3} \).

Later Arndt (1996) adapted Stroud’s formulae for multivariate standard normal distributions by adjusting the size of the region of integration:

Let \( \Gamma_k \) denote the point \((\gamma_1, \gamma_2, \ldots, \gamma_n)\) where

\[
\gamma_{2r-1} = \sqrt{2} \frac{\cos \left(\frac{(2r-1)k\pi}{n}\right)}{n} \quad \gamma_{2r-1} = \sqrt{2} \frac{\sin \left(\frac{(2r-1)k\pi}{n}\right)}{n} \quad r=1,2,\ldots,\left[\frac{n}{2}\right],
\]

if \( n \) is odd \( \gamma_n = (-1)^k \).

As demonstrated in figure 2, the initial position from where we start the rotation of Stroud’s octahedron impacts the accuracy of the results produced by Gaussian Quadratures. The initial position is determined by the arrangement of the covariance matrix of the stochastic variables. Since up to this point there is no generic method developed of how to select the initial position of the octahedron that gives the most accurate quadrature points we suggest to randomly choose \( k \) (\( k \leq n! \)) number of initial positions and perform rotation for each of the \( k \) initial situations. This will give us \( k \times 2n \) Gaussian quadrature points, where \( n \) is the number of stochastic variables, consequently producing \( k \times 2n \) series of results. We believe that
calculating the 1\textsuperscript{st} (means) and the 2\textsuperscript{nd} (standard deviations) moments from the \( k \times 2n \) series will lead to more reliable results than calculating these for \( 2n \) series only.

**Data**

Since in 2011 Sudan was divided into 2 states: the Sudan and South Sudan, we had no separated data prior to that date.

Therefore, we have obtained the regionally disaggregated data for the Sudan for the period of 1981-2011 and have aggregated them based on the production shares. The following crops are treated stochastically: irrigated cotton, irrigated, mechanized rainfed and traditional rainfed sorghum, irrigated wheat, irrigated groundnuts, mechanized rainfed and traditional rainfed millet, mechanized rainfed and traditional rainfed sesame. Fig. 4 presents the historical yield data of the stochastically treated crops:

![Fig. 4: Aggregated historical yield data. Source: own development.](image)

The detrending and the separation of the stochastic components of the data have been performed following the methodology of Burrell & Nii-naate (2013) which states that if the historical time series are stationary the deviations from the mean should be taken and if the data are trended the deviations from the time trend should be considered. The deviates are captured as shares following the below-given formula, where \( Z_i \) is the deviate or the stochastic component of the \( i \)\textsuperscript{th} year, \( y_i \) is the observed historical data of the \( i \)\textsuperscript{th} year, \( \hat{y}_i \) is the estimated trend value of the same year and if the data are stationary \( \hat{y}_i \) is the mean of the historical data:

\[
Z_i = \frac{y_i}{\hat{y}_i} - 1
\]
By this approach, we obtain a series of deviates (or stochastic components) with an expected mean value of 0 and a standard deviation within the interval of (0:1).

Table 1 presents the correlation matrix of the deviates of yield data from the estimated trends:

<table>
<thead>
<tr>
<th></th>
<th>cotton_irr</th>
<th>groundnuts_irr</th>
<th>millet_rain</th>
<th>sesame_rain</th>
<th>sorghum_irr</th>
<th>sorghum_rain</th>
<th>wheat_irr</th>
</tr>
</thead>
<tbody>
<tr>
<td>cotton_irr</td>
<td>1</td>
<td>0.200</td>
<td>0.101</td>
<td>0.103</td>
<td>-0.296</td>
<td>-0.052</td>
<td>-0.280</td>
</tr>
<tr>
<td>groundnuts_irr</td>
<td>0.326</td>
<td>1</td>
<td>0.349</td>
<td>0.230</td>
<td>0.032</td>
<td>-0.281</td>
<td></td>
</tr>
<tr>
<td>millet_rain</td>
<td>0.141</td>
<td>1</td>
<td>0.045</td>
<td>0.447</td>
<td>-0.351</td>
<td></td>
<td></td>
</tr>
<tr>
<td>sesame_rain</td>
<td>0.167</td>
<td>1</td>
<td>0.052</td>
<td>-0.209</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>sorghum_irr</td>
<td>0.155</td>
<td>1</td>
<td></td>
<td>0.019</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>sorghum_rain</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>wheat_irr</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>1</td>
</tr>
</tbody>
</table>

Table 1: correlation matrix of the deviates from linear trends.

**Modeling**

We use an economy-wide modeling suite that comprises the IMPACT Model System (Robinson et al. 2015) linked to biophysical modules, including hydrology, river basin management, crop water stress and crop simulation models in addition to a recursive dynamic CGE model (Al-Riffai et al., 2017). The dynamic CGE model is calibrated to the most recent post-separation social accounting matrix (SAM) for the Sudan (Siddig et al. 2016). For the period of 2018-2050, we apply two scenarios: no climate change scenario (NoCC) and combined climate change scenario (ComCC1) depicting two different developments of the climate change and their impact on yields. The NoCC scenario assumes that the climate change will have no impact on yields (business as usual) and is the baseline scenario to which the results from the other scenario will be compared. The ComCC1 scenario is the combination of both local and global climate change impacts. The yield changes according to the above-mentioned scenarios are calculated by the IMPACT model and are applied in the CGE as annual TFP shocks.

Since extreme weather shocks in Sudan occur in a cyclical manner – every 5 years, the stochastic shocks are applied in every 5th year starting from 2018 (7 times for the period of 2018-2050). Following the approach of increasing the reliability of the GQ approximation explained above we randomly permute the arrangement of the covariance matrix 20 times, which gives us 20 series of stochastic shocks. However, since we are dealing with a recursive dynamic model setup and each series of the stochastic shocks should be applied 7 times we face a risk of applying the same stochastic shock (positive or negative) 7 times in a row for each iteration. Therefore, in order to avoid this, after randomly arranging the covariance matrix 20 times, in each of these randomly arranged matrices, we select the vector with the highest coefficient of variation (CV)² and permute it 7 times in the given matrix setup. This process is described in fig. 5:

---

² CV = (standard deviation/mean) * 100
This way we are able to obtain 20 randomly generated series of Gaussian quadrature points and to avoid the risk of applying the same stochastic shocks with the same sign 7 times in a row in each iteration.

**Results**

The results are analyzed from the angle of differences in the results produced by different random rotation of Stroud’s octahedron. Due to the fact that the model applied here is large in terms of the number of functions to be solved and that it is recursive dynamic which adds an additional time dimension to the model having a multiplicative impact on the model dimensionality, it was not possible to obtain converged results using Monte Carlo approach, even though we used a powerful computational cluster. This is also the case for most of the large-scale simulation models trying to apply Monte Carlo approach, therefore, the sample sizes of MC points applied are mostly not validated and relatively small for obtaining accurate results (e.g. Valin et al. (2015); OECD-FAO (2017); Artavia et al. (2015), etc.). Therefore, our intention here is to demonstrate how the proposed method of decreasing the inaccuracies produced by different rotations of Stroud’s octahedron behaves.

The results are presented by the real crop GDP values under both “no climate change” and “combined climate change” scenarios. Looking at the first moments of the crop GDP (figure 6) we don’t see any differences among the results produced by different GQs at this scale. However, if we zoom in the results and by following the approach by Arndt & Thurlow (2015) observe the average of the results of the final 5 year period (2046-2050) of each rotation, assuming that the final five years will include the cumulative effects of all the shocks applied during the preceding years, we will notice quite some inaccuracies (figure 7). And since the only information we have about the true value is that it lies somewhere in between of those 20 values we suggest that by taking the mean of the results received by the 20 rotations will reduce the risk of possible inaccuracies caused by the choice of the GQs.
The second moments are represented by the coefficient of variations (CV):

\[ CV = \frac{\sigma}{\mu} \times 100 \]

In this context, the measure can be interpreted as the risk of volatility of a specific variable. So the higher this value for a variable is, the larger is the risk of volatility around it.

As expected, some inaccuracies occur while estimating the second moments of the distributions. Here the impact of different matrix arrangements is more prominent. Figure 8 presents the annual CVs of real crop GDP evaluated by 20 random rotations of Stroud’s octahedron and the mean on these 20 developments is presented by the black dashed line.
Again if we observe the average coefficient of variations of the final 5 years (figure 9) we will notice that the relative differences between the results produced by different rotations are high, considering that the highest result (P9) among the ones received by 20 random rotations of Stroud’s octahedron is almost double the lowest result (P14).

Then we decided to check how well is the proposed approach able to depict the distribution of the results compared with a single rotation. For that purpose, we randomly selected one year (in this case year 2034) and plotted the pdf given the number of points from each case (figure 10). In case of a single rotation, in order to evaluate the integral, we used 14 quadrature points, consequently if we rotate Stroud’s octahedron 20 times the number of quadrature points will be 280. Figure 10 illustrates that by incorporating a random component...
into the GQ method we manage to create a distribution of results (including the tails) compared the previously known discrete approximation method.

PDF Crop GDP, 2034. 20 rotations

PDF Crop GDP, 2034. 1 rotation

Fig. 10
Conclusions and Remarks

Artavia et al. (2015) was the first study that drew attention to the fact that different rotations of Stroud’s octahedron impact the accuracy of the approximation, although the literature existing prior to this study (e.g. Preckel et al. 2010) had persistently denied this fact. For the last two years, we have observed the same phenomenon by testing the methodology in various toy models\(^3\) with different dimensionalities and different levels of asymmetries. However, the accuracy of each rotation is unique in each model, therefore, up until now, there are no clear guidelines on which exact rotation produces the most accurate results given the specific model characteristics. Having this in mind, in this paper we present an approach that will decrease the risk of getting inaccurate results while using the GQ methodology, which in contrast to the computationally burdensome Monte Carlo method requires a minimum number of points to evaluate the numerical integral (C. Arndt, 1996). Villoria & Preckel (2017) criticized the GQ approach emphasizing the fact that GQs poorly depict the 3rd moments of the distribution compared with the Monte Carlo method. While predominantly agreeing with this statement we want to point out that the GQ is a numerical integration method of degree 3 and principally is only suitable for approximating the means and variances of a given distribution (Stroud, 1957). In this light, we once more draw your attention to figure 10 which principally implies that the proposed methodology has a potential of producing more accurate approximations of higher moments.

The future work will be devoted to finding an algorithm that will give the optimal number of random rotations of Stroud’s octahedron required in order to minimize the approximation error of the proposed approach given the specific model factors and characteristics. We will also strive to identify the exact model characteristics affecting the accuracy of the GQ method, in order to be able to choose the right rotation of Stroud’s octahedron for a specific model setup.

\(^3\) In order to be able to set up a benchmark with converged Monte Carlo approximation to which the results obtained by GQ approach have been compared.
References


