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Multiple Rotations of Gaussian Quadratures: An Efficient Method for Uncertainty Analyses in Large-Scale Simulation Models

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Abstract

Concerns regarding the impacts of climate change, food price volatility and uncertain macroeconomic conditions have motivated users of large-scale simulation models addressing agricultural markets to consider uncertainty in their projections. One way to incorporate uncertainty in such models is the integration of stochastic elements, thus turning the model into a problem of numerical integration. In most cases, such problems do not have analytical solutions, and researchers apply methods of numerical approximation. This article presents a novel approach to uncertainty analysis as an alternative to the computationally burdensome Monte Carlo or quasi-Monte Carlo methods, also known as probabilistic approaches. The method developed here is based on Stroud's degree three Gaussian quadrature (GQ) formulae. It is tested in three different large-scale simulation models addressing agricultural markets. The results of this study demonstrate that the proposed approach produces highly accurate results using a fraction of the computation capacity and time required by probabilistic approaches. The findings suggest that this novel approach, called the multiple rotations of Gaussian Quadratures (MRGQ), is highly relevant to increasing the quality of the results since individual GQ-rotations tend to produce results with rather large variability/approximation errors. The MRGQ method can be applied to any simulation model, but we believe that the main beneficiaries will be users of large-scale simulation models who struggle to apply probabilistic methods for uncertainty analyses due to their high computational, data management and time requirements.

Keywords: Uncertainty analysis, stochastic modeling, multiple rotations of Gaussian Quadratures, MRGQ, efficient formulae, Latin Hypercube sampling, Monte Carlo sampling, probabilistic formulae, computable general equilibrium modeling, partial equilibrium modeling.

1. Introduction

Simulation models are an established tool for assessing the impacts of exogenous shocks on economic, social and ecological systems. They are also widespread in analyses of agricultural systems and land use. Yet, since all models are imperfect representations of real-world systems and accurate input data is not always available, the robustness of model results remains an issue to be addressed. In addition, the uncertainty of model results due to the real-world volatility of variables such as weather is often a subject of analysis itself.

A standard approach to tackling uncertainty in large-scale simulation models depicting agricultural markets is the incorporation of stochastic terms. This approach opens a path for addressing not only issues of robustness, but also a wide range of policy questions related to uncertainty. Stochastic analyses can be classified into two main groups, depending on their purpose. First, there are analyses that apply stochastic modeling features in order to perform systematic sensitivity analyses regarding unknown model parameters (Arndt and Hertel 1997; Valenzuela et al. 2007; Beckman et al. 2011; Villoria et al. 2013). Second, there are analyses which consider explicitly the uncertainties inherent in input variables such as weather by describing these variables with probability distributions and producing distributions of model outputs under input uncertainty (OECD-FAO Agricultural Outlooks in the last decade; European Commission 2018). The latter are known as uncertainty analyses (Loucks and Van Beek 2005). In the simulation of agricultural systems, many studies address the policy implications of uncertainty (Westhoff et al. 2005; Moss et al. 2010; Hertel et al. 2010; Verma et al. 2011; Gouel and Jean 2013).

In order to solve stochastic simulation models, researchers normally apply numerical approximation methods since such problems in most cases do not have analytical solutions (Arndt 1996). Two of these approximation methods are applied widely in stochastic simulation modeling:

Monte Carlo (MC) or quasi-MC methods, and Gaussian Quadratures (GQ) (Artavia et al. 2015). The MC approach typically demands large computational capacity requiring thousands of iterations for each stochastic variable or parameter (Haber 1970). In contrast, GQ requires a minimal number of iterations ($2n$, where n is the number of stochastic variables and parameters) to reproduce the second central moments of a joint probability distribution. However, recent studies have pointed out potential inaccuracies in results approximated by GQ resulting from the heterogeneous quality of different quadratures as well as its weak approximation of the tails of distributions (Artavia et al. 2015; Villoria and Preckel 2017).

In this article, a novel approach to the approximation error reduction for GQ, called multiple rotations of Gaussian Quadratures (MRGQ), is presented as a means for conducting affordable and accurate uncertainty analyses in large-scale simulation models. The MRGQ works best in cases of symmetric distributions, e.g. Gaussian or triangular, however can also be adjusted to cases of skewed distributions of input parameters via the method of DeVuyst and Preckel (2007). The proposed MRGQ method is tested in three large-scale simulation models (both partial and general equilibrium) depicting agricultural markets: A comparative static computable general equilibrium (CGE) model applied to Bhutan, a global partial equilibrium (PE) model, and a recursive dynamic CGE model applied to the Sudan.

The remainder of this article is organized as follows: Section 2 gives a short overview of the theoretical backgrounds of the most widely used methods of stochastic modeling. Next, Section 3 introduces the applied approach for generating a benchmark against which the quality of the approximations made by GQ and the proposed MRGQ method will be evaluated. Section 4 provides an overview of the simulation models and data, while Section 5 presents the benchmark

results and the approximation results generated by GQ and MRGQ. Finally, Sections 6 and 7 offer a discussion and conclusions.

2. Stochastic modeling as a numerical integration problem

Let us consider a simple example of an uncertainty analysis in a simulation model. Let x be an exogenous variable or parameter, g(x) the probability density function describing the uncertainty of x supported on some interval [a, b], and f(x) some function in the model for which we want to find the expected value

$$(1)\quad E[f(x)] = \int_a^b f(x)g(x)dx .$$

In many applications, such integrals cannot be evaluated directly since they are not given in closed form. Instead, numerical integration methods must be employed. To this end, we choose n points x_k within the domain of integration, the so-called nodes, with associated weights w_k, and approximate the integral (1) by the finite sum

$$(2)\quad \tilde{E}[f(x)] = \sum_{k=1}^n f(x_k)w_k .$$

Usually, the nodes and their weights for such a quadrature formula are chosen in such a way that the approximation (2) yields the same results as (1) at least for polynomials of low degree. Therefore, the degree of accuracy of the quadrature formula (2) is defined as

$$(3)\quad \max\{M \in N_0 : E[x^m] = \tilde{E}[x^m] \text{ for } m = 0,...,M\} .$$

It is worth noting that this approach amounts to approximating the continuous probability distribution with density function g(x) in (1) by a finite discrete probability distribution, where the latter is chosen in such a way as to share as many moments (expected value, variance, skewness, kurtosis, ...) with the former as possible.

This approach can also be used for multivariate integrals; then we refer to approximations of type (2) as cubature formulae. As an example, consider the case of the multivariate normal distribution with mean vector $\vec{\mu}$ and covariance matrix Σ. Then $g(\vec{x})$ is given by

$$(4) \quad g(\vec{x}) = \frac{1}{\sqrt{(2\pi)^d \det(\Sigma)}} \exp\left(-\frac{1}{2}(\vec{x}-\vec{\mu})^T \sum{}^{-1}(\vec{x}-\vec{\mu})\right)$$

Note, however, that this implies that the domain of integration is not bounded anymore, but instead is all of R^n.

There exist a wide range of methods for choosing the nodes and their weights; the ones used most frequently belong to one of the following two main classes: probabilistic formulae and efficient formulae.

2.1. Probabilistic formulae

This category of formulae includes the well-known MC method and all related variance reduction approaches, also known as quasi-MC methods (Haber 1970). The basic idea behind this group of methods is to perceive of the integration as a probabilistic problem and solve it approximately using statistical experiments. Therefore, the underlying logic is to choose the nodes randomly. Then, according to the law of large numbers, we may expect the numerical result to be close to the correct value if the number of points is sufficiently large.[1] Although those methods are easy to apply and very effective, they are not efficient, as they require large sample sizes. For example, according to Haber (1970), the MC sample size should range from 40,000 to 100,000 in order to obtain an error below 1%. Therefore, the main disadvantages of this group of methods are the slow convergence rates (Engels 1980) and high computational requirements. Since a sufficient number

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[1] Throughout this paper, we refer to the process of better approximating the true distribution by a larger sample size as convergence.

of iterations is necessary for obtaining reliable results (Arndt 1996), their application in large-scale simulation models becomes very expensive, if not infeasible, in terms of the computational requirements, time, and data management costs.

Quasi-MC approaches incorporate features of stratified sampling with the characteristics of random sampling. This strategy has several advantages over pure random sampling. First of all, it ensures that the randomly selected points are spread somewhat evenly across the domain of the distribution according to the probability mass, thus increasing the rate of convergence considerably. Hence, the sample size required to obtain results of equal quality is much smaller than in random sampling. The Latin Hypercube sampling (LHS) technique is one approach to incorporate random sampling and stratification. It divides the domain of the probability distribution into N subsets of equal probability, where N is the sample size, and then randomly picks one point from each subset (Helton and Davis 2003). Since there is no predetermined sample size that fits all models, very often and frequently driven by computational feasibility, uncertainty analyses in large-scale simulation models are performed using ad hoc and relatively small sample sizes that might limit the quality of the approximations (e.g., Mary et al. 2018; OECD-FAO 2017; Valin et al. 2015; Villoria and Preckel 2017).[2]

2.2. Efficient formulae

As suggested by the name, this group of formulae aims at obtaining results with a certain degree of exactness using the least possible number of points. In this section, we refer to degree three quadrature formulae by Stroud (1957), whose theorem 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

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[2] Those studies apply 550, 190, 300 and 10,000 points, respectively.

vertices of a Q_n whose centroid coincides with the centroid of the region and lie on an n-sphere of radius $r = \sqrt{nI_2 / I_0}$ " (Stroud 1957, p. 259).

Here, Q_n is the regular, n-dimensional generalized octahedron being integrated into the n-sphere, I_0 is the volume of the symmetrical region and I_2 is the integral of the square of any of the variables of the region over the entire region. Figure 1 is a graphical representation of the theorem. In other words, the theorem states that in order to obtain an n-dimensional Gauss quadrature formula of degree three for an n-dimensional cube, we have to use 2n points that are the vertices of a regular n-octagon (points 1-6 in figure 1) whose centroid is the centroid of the cube. If those conditions are met, an approximation with exactness of order three can be obtained.
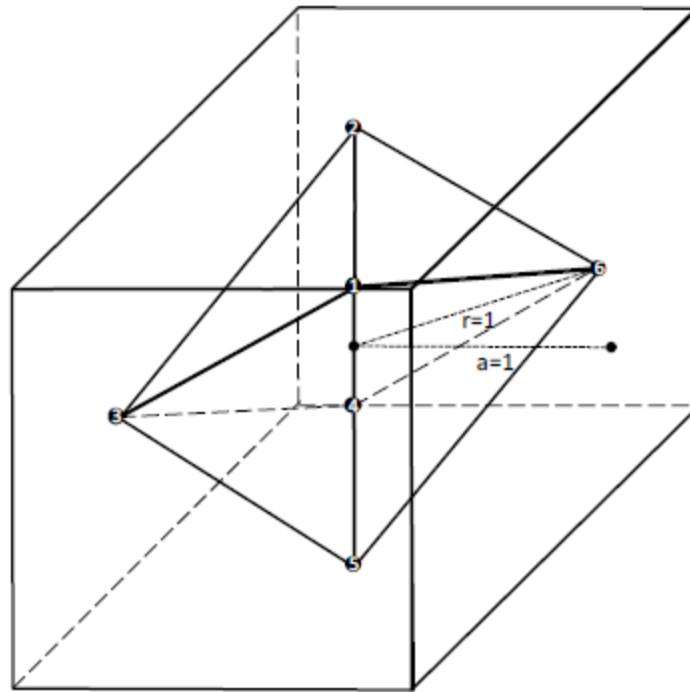

Figure 1. Graphical representation of Stroud's theorem for the degree three quadrature formulae.
Notation: a- vertice of the n-sphere, r - radius of the n-octahedron.
Source: Artavia et al. (2015).

However, Stroud was faced with the problem that whenever the dimensionality is greater than three, the vertices fall outside of the integration region and therefore yield unusable formulae. This problem can be observed in the calculation below, which is adopted from Artavia et al. (2015). The volume of an n-cube (C^n) with vertices ($\pm a, \pm a,..., \pm a$) can be obtained as follows:

$$(5) \quad I_0 = \int_{C^n} x_i^0 d\vec{x} = (2a)^n$$

The integral of the square of any variable over this region is:

$$(6) \quad I_2 = \int_{C^n} x_i^2 d\vec{x} = \int_{C^{n-1}} d\tilde{\vec{x}} \int_{[-a,+a]} x_i^2 dx_i = (2a)^{n-1} \left[\frac{1}{3} x_i^3 \right]_{-a}^{+a} = (2a)^{n-1} \frac{2}{3} a^3 = \frac{2^n}{3} a^{n+2}.$$

Here, $\tilde{\vec{x}} \in R^{n-1}$ is the vector $\vec{x}$ with the coordinate x_i omitted.

Thus yielding the radius of the octahedron:

$$(7) \quad r = \sqrt{n \frac{I_2}{I_0}} = \sqrt{n \left(\frac{2^n}{3} a^{n+2} / 2^n a^n \right)} = \sqrt{n \frac{a^2}{3}} = a \sqrt{\frac{n}{3}}.$$

In the case depicted in figure 1, we deal with a three dimensional cube with the vertices ($\pm 1, \pm 1, \pm 1$), and for n = 3, we obtain r = 1.

As a solution for this problem, Stroud (1957) suggested the following formulae to rotate the octahedron in order to bring the quadrature points back into the integration region. For k = 1,...,2n, let Γ_k denote the quadrature point $(\gamma_{k,1}, \gamma_{k,2},..., \gamma_{k,n})$, where:

$$(8) \quad \gamma_{k,2j-1} = \sqrt{\frac{2}{3}} \cos\left(\frac{(2j-1)k\pi}{n} \right)$$

$$(9) \quad \gamma_{k,2j} = \sqrt{\frac{2}{3}} \sin\left(\frac{(2j-1)k\pi}{n} \right)$$

for $j = 1,..., \left[\frac{n}{2} \right]$, where $\left[\frac{n}{2} \right]$ is the greatest integer not exceeding $\frac{n}{2}$; in addition, if n is odd:

$$(10)\ \gamma_{k,n} = \frac{(-1)^k}{\sqrt{3}}$$

The quadrature points generated by these formulae fulfil the above-mentioned three prerequisites.

Arndt (1996) adapted Stroud's formulae for integrals over all of R^n (Euclidian space) with the multivariate standard normal distribution as a weight function. Arndt's formulae are just the Stroud points multiplied by $\sqrt{3}$, which follows from the fact that the value of the radius $\left(r = \sqrt{n\frac{I_2}{I_0}} \right)$ changes:

$$(11)\ I_0 = \int_{R^n} x_i^0 \frac{1}{(2\pi)^{n/2}} e^{-\frac{\|\vec{x}\|^2}{2}} d\vec{x} = (1)^n = 1$$

$$(12)\ I_2 = \int_{R^n} x_i^2 \frac{1}{(2\pi)^{n/2}} e^{-\frac{\|\vec{x}\|^2}{2}} d\vec{x} = \int_{R^{n-1}} \frac{1}{(2\pi)^{(n-1)/2}} e^{-\frac{\|\tilde{\vec{x}}\|^2}{2}} d\tilde{\vec{x}} \int_R x_i^2 \frac{1}{(2\pi)^{1/2}} e^{-\frac{x_i^2}{2}} dx_i = (1)^{n-1} 1 = 1.$$

Here, $\|\vec{x}\|$ denotes the Euclidean norm of the vector $\vec{x} \in R^n$, and $\tilde{\vec{x}} \in R^{n-1}$ is the vector $\vec{x}$ with the coordinate x_i omitted; so, in particular, $\|\vec{x}\|^2 = \|\tilde{\vec{x}}\|^2 + x_i^2$.

It follows that

$$(13)\ r = \sqrt{n\frac{I_2}{I_0}} = \sqrt{n}$$

Therefore, equations (8) to (10) have to be adapted accordingly, and for the kth quadrature point $\Gamma_k = \left(\gamma_{k,1}, \gamma_{k,2}, ..., \gamma_{k,n} \right)$, where k = 1, 2,…, 2n, we obtain:

$$(14)\ \gamma_{k,2j-1} = \sqrt{2} \cos\left(\frac{(2j-1)k\pi}{n} \right)$$

$$(15)\ \gamma_{k,2j} = \sqrt{2} \sin\left(\frac{(2j-1)k\pi}{n} \right)$$

for $j = 1,..., \left[\dfrac{n}{2}\right]$, where $\left[\dfrac{n}{2}\right]$ is the greatest integer not exceeding $\dfrac{n}{2}$, and if n is odd:

$$(16)\ \gamma_{k,n} = \left(-1\right)^{k}$$

In order to endow the finite distribution with the desired covariance matrix Σ, we need to multiply the sampling points with a square matrix A satisfying $\Sigma = AA^{T}$. There are a number of standard methods that can be used to obtain A from Σ, such as eigenvalue decomposition, Cholesky factorization, reverse Cholesky factorization, and so forth (Artavia et al. 2015). Therefore, the matrix of the final quadrature points $\left(\Psi\right)$ can be obtained as follows: $\Psi = \vec{\mu} + \Gamma A$, where $\vec{\mu}$ is the vector of mean values (e.g., the base values of parameters). In this study, we use the eigenvalue decomposition technique.

After the method of GQ had been used for many years as a means of uncertainty analysis in many large-scale simulation models (e.g., Arndt and Hertel 1997; Valenzuela et al. 2007, Villoria et al. 2013), Artavia et al. (2015) found that depending on the initial position of the octahedron from which the rotation starts, the quality of the approximation differs. In addition, a recent study by Villoria and Preckel (2017) pointed out inaccuracies in the GQ in the Global Trade Analysis Project (GTAP) model. Namely, they compared the results produced by GQ with the ones obtained by MC and discovered large differences in the first three moments of the probability distributions. In this article, we present a novel approach, termed MRGQ, in order to deal with this issue.

3. Methods

3.1. Benchmark generation

In the first step, we generate a reliable benchmark against which the results obtained by the proposed MRGQ method will be compared. We use the well-established LHS technique and systematically determine a sufficient sample size for each model. To this end, we solve each model using the LHS technique with a converged sample size, meaning that we start solving the model

11

with a small sample size, then gradually increase it[3] and observe the behavior of the coefficients of variation (CV) of two variables: the total production of each crop for which the productivity was shocked, and the respective price levels.[4] The stop criterion is satisfied when the percentage change in the results of interest compared to the results from the previous sample size stay within a [-1%, 1%] interval. The advantages of using the CVs as an indicator are twofold: first, this measurement is dimensionless, thus facilitating comparison, and second, it captures both the first and the second moments of the data.

3.2. MRGQ method

Artavia et al. (2015) showed that the quality of the GQ results depends strongly on the selected rotation of Stroud's octahedron. In order to counteract this effect, we use several families of GQ points generated from different random rotations of Stroud's octahedron. To this end, we randomly choose k of the n! possible permutations of the n coordinates before applying the Stroud matrix. Doing so increases the number of quadrature points by a factor of k but, at the same time, improves the quality of the output drastically, as will be shown in the results section.

Following the insights of Artavia et al. (2015), we also investigate how the initial position of Stroud's octahedron from which we start the rotation affects the final results of the GQ approximation. We generate ten series of quadratures via ten random rotations of the octahedron for the GLOBIOM model and 20 series by 20 random rotations for each of the other two models. Note that each series contains only 2N points, where N is the number of stochastically treated variables. The number of random rotations is selected arbitrarily, considering the available computational capacities. After solving the models with the quadrature points generated by each

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[3] For all models, we use sample sizes of 1,000 and 2,000 as well as further increases in sample sizes in steps of 2000. Depending on the complexity of the model, we use sample sizes below 1000 as ad hoc choices.
[4] These two variables are selected for demonstration purposes. Generally, the variables most relevant to the respective study should be selected.

individual rotation, we also solve them using the MRGQ method. The quality of the MRGQ method is then evaluated against the generated benchmark. In the case of the Dynamic CGE, we follow the approach of Arndt and Thurlow (2015) and observe the final five-year average of the results only, assuming that doing so will allow us to capture the cumulative effects of the stochastic shocks from previous time periods.

4. Simulation models and data

The MRGQ approach is tested in three different simulation models: 1) a comparative-static, single-country CGE model based on the Static Applied General Equilibrium Model (STAGE Version 2) (McDonald and Thierfelder 2015) and extended for, and applied to, Bhutan (Feuerbacher et al. 2018) (named "Static CGE" throughout this article); 2) GLOBIOM (Havlík et al. 2011; Havlik et al. 2014), which is a global partial equilibrium model for the agricultural and forestry sectors; and 3) a multi-sector recursive-dynamic CGE model for the Sudan (Diao and Thurlow 2012) (named "Dynamic CGE" throughout this article). All three models are programmed in the General Algebraic Modeling System (GAMS) modeling language.

In all three models, we test the uncertainty of crop yields, which is a major determinant of agricultural price volatility. For that purpose, we have obtained historical data from FAOSTAT (2018), ICRISAT (2018) and national agencies/institutions (MoAF 2016). Then, following the procedure used by Burrell and Nii-naate (2013), when sufficient data is available, we separate the stochastic components of the historical yield data for the crops as deviates from the estimated trends based on which the stochastic points are generated. Since the expected value of the stochastic shocks is equal to zero, the choice of the crops whose yields are to be stochastic is not important in this context.[5]

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[5] In this article, the choice of stochastic yield variables is related to the data quality and availability.

4.1. The Static CGE

The Static CGE is a single-country, comparative-static CGE model using the STAGE2 framework which is documented extensively in McDonald and Thierfelder (2015). The Static CGE extends the basic STAGE2 model to include a multi-level production structure of nested Constant Elasticity of Substitution (CES) and Leontief fixed-coefficient technologies. Furthermore, the demand system follows a two-stage Linear Expenditure System (LES) -CES nest allowing for the substitution of commodities within commodity groups. The model extension and parameters are documented in Feuerbacher (2019). The model is calibrated to a 2012 social accounting matrix for Bhutan (Feuerbacher et al. 2017) with multiple sectors, ten of which are crop-producing sectors. The model is run in an investment-driven setup, i.e., household saving rates adjust to meet a given level of investments. The exchange rate is flexible, and foreign savings are fixed. Reflecting the short-term nature of the stochastic shock, the model closures account for fixed land allocation (no land mobility across crop sectors), fixed government spending and flexible government savings (all tax rates remain constant). The impact of the yield uncertainty is evaluated for all ten crop-producing sectors comprising of: paddy, maize, wheat, pulses, vegetables, potatoes, spices, apples, citrus fruits and other fruits and nuts. Stochastic changes in crop yields are modeled by shocking the respective crop sector's total factor productivity.

4.2. GLOBIOM

GLOBIOM is a bottom-up, recursive-dynamic partial equilibrium model with global coverage integrating the agricultural, bioenergy and forestry sectors (Havlík et al. 2011; Havlik et al. 2014). It is a linear programming model with a spatial equilibrium approach (Takayama and Judge 1971). The market equilibrium for agricultural and forestry products is computed based on a welfare maximizing objective function subject to resource, technology, demand and policy constraints.

The model version applied in this article covers 31 regions globally and considers the 18 most important crops in terms of globally harvested quantities. Since this version of the model already requires a large computational capacity, we use it in a comparative static framework, starting from a fixed 2010 solution and solving the model only for one time step (2020). We analyze the yield uncertainties of Indonesia and Brazil. The uncertainty of the following crops is tested in each region: 1) Indonesia- groundnuts, maize, rice, soybeans and sugarcane; and 2) Brazil- barley, groundnuts, sorghum, potatoes, dry beans, rice, wheat, sugarcane, maize, soybeans, cassava and sweet potatoes.

4.3. The Dynamic CGE

The Dynamic CGE is an economy-wide, recursive-dynamic CGE model (Diao and Thurlow 2012) linked to the IMPACT modeling system (Robinson et al. 2015). The model is calibrated to the most recent social accounting matrix for the Sudan with multiple sectors, 26 of which are crop producing (Siddig et al. 2016). The demand for primary factors is governed by CES functions, while the intermediate input demand is determined by Leontief fixed-coefficient technology. As in the Static CGE, we assume government savings to be flexible, whereas direct tax rates are fixed. For the external balance, a flexible exchange rate is chosen, while the foreign savings are fixed. Finally, for the saving-investment identity, a fixed share of investment in absolute absorption is assumed, while endogenously adjusting household saving rates in a uniform way, in order to generate the necessary funds.

The uncertainty of the following crop yields is analyzed in the context of the Dynamic CGE: irrigated cotton, irrigated and mechanized rain-fed sorghum, irrigated wheat, irrigated groundnuts, mechanized rain-fed millet, and mechanized and traditional rain-fed sesame. Although the recursive-dynamic framework of the model is set up to project for the period of 2018 to 2050, we

conduct our study for the time interval 2018 to 2025 in order to be able to obtain a benchmark, considering the huge computational requirements of the LHS approach. Since extreme weather shocks in Sudan occur in a cyclical manner (MEPD 2013), on average every five years, the stochastic shocks are applied in every fifth year; in this case, in 2018 and 2023.

5. Results

In the following two sub-sections, the benchmark results for each model and the results generated by the proposed MRGQ method are presented.

5.1. Benchmark

The Static CGE as a single-country CGE model in comparative-static mode represents a model category that, unlike the other two models, is characterized by relatively low computational requirements. In the case of production quantities, we obtain convergence at 10,000 iterations, yet, for reaching convergence in prices, the number of points must be increased to 20,000 (figures 2a, 3a). Therefore, the sample size of 20,000 iterations is selected as the benchmark.

For GLOBIOM, the number of iterations is raised up to 10,000. However, at that point, we do not yet reach convergence for all crops: four out of the 17 price variables are still exhibiting changes slightly above the 1% threshold. Yet, given the resources required to continue increasing the number of iterations (approximately 3,000 computer-hours for 12,000 iterations), we accept the results of 10,000 iterations as a benchmark since the majority of the crops converge at that point for both analyzed variables (figures 2b, 3b).

For the Dynamic CGE, we evaluate convergence by analyzing the behavior of the mean absolute CVs of the growth rates of production and prices over the projected period. For the production growth rates, we obtain convergence at 14,000 iterations, whereas convergence for the growth

rates of prices is reached at 12,000 points (figures 2c, 3c). Thus, 14,000 iterations is chosen as benchmark for the Dynamic CGE model.

In figure 2, one can also observe that model dimensionality and complexity are positively correlated to the relevance of increasing the sample size for reaching CV convergence.
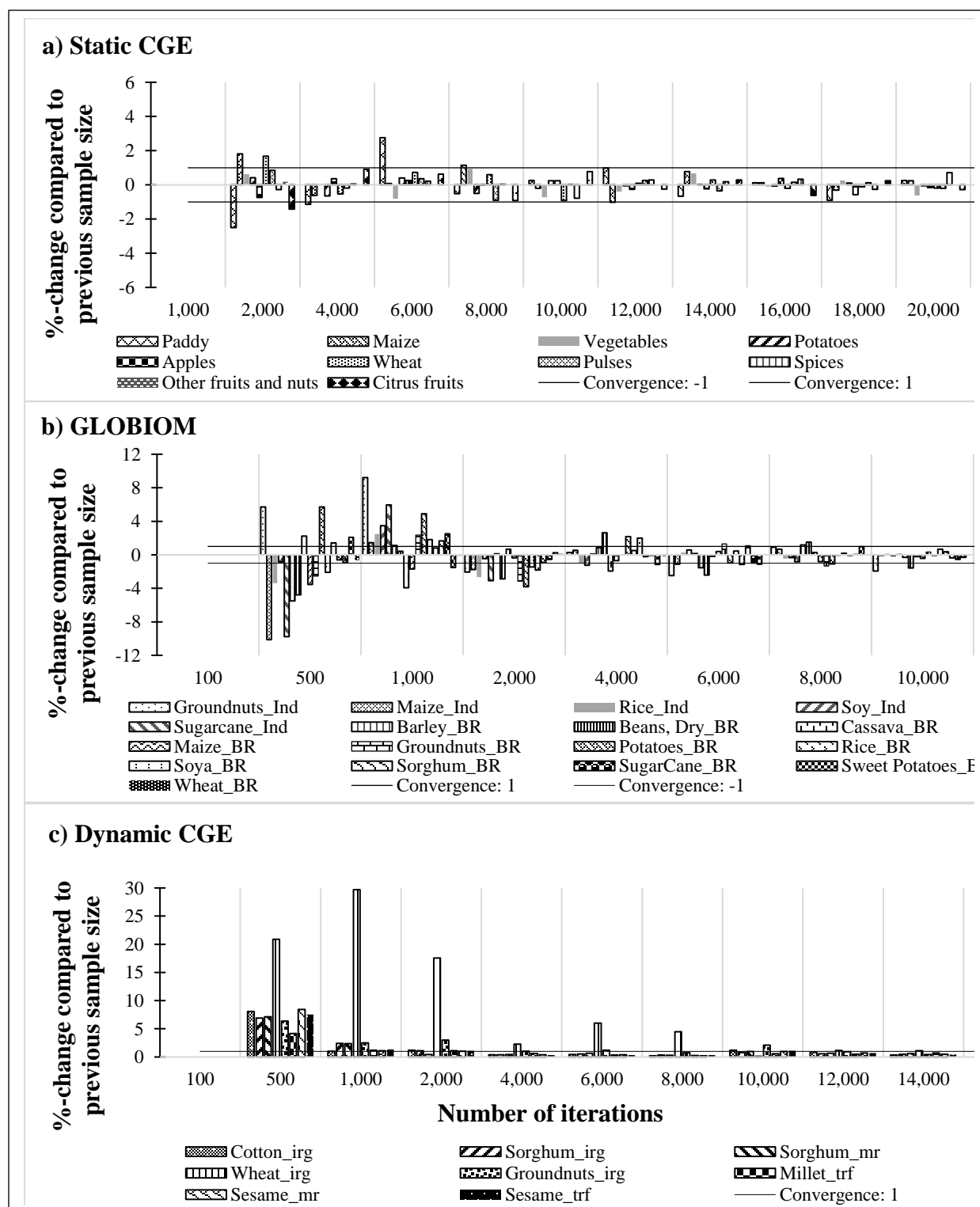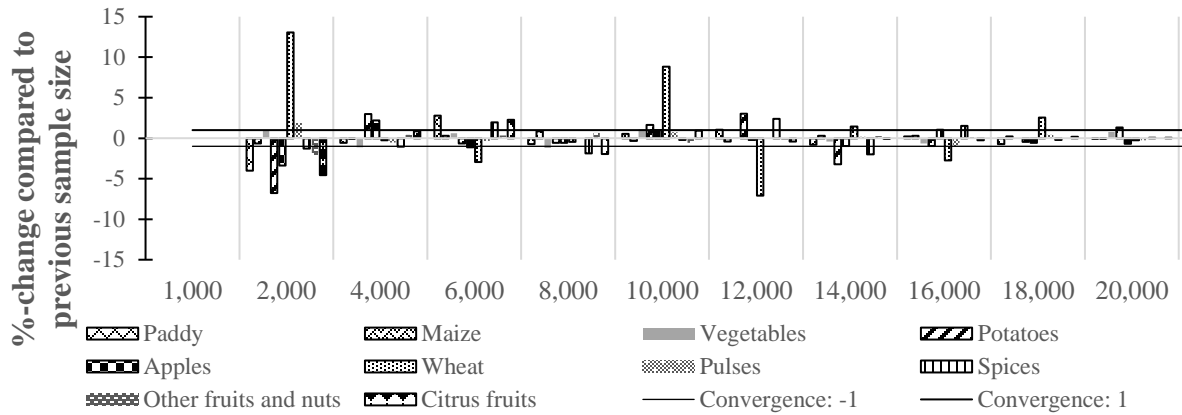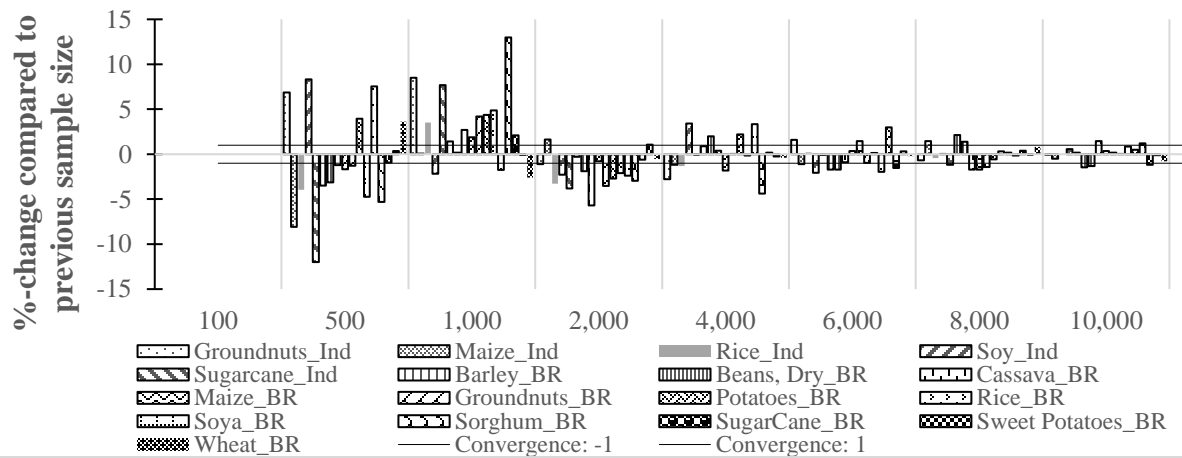
Figure 2. Convergence of the CVs of the production quantities for the (a) Static CGE and (b) GLOBIOM models and of the average absolute production growth rate over the projected period for the (c) Dynamic CGE model.

Notation: Ind-Indonesia, BR-Brazil, irg-irrigated, mr- mechanized rain-fed, trf- traditional rain-fed.

a) Static CGE
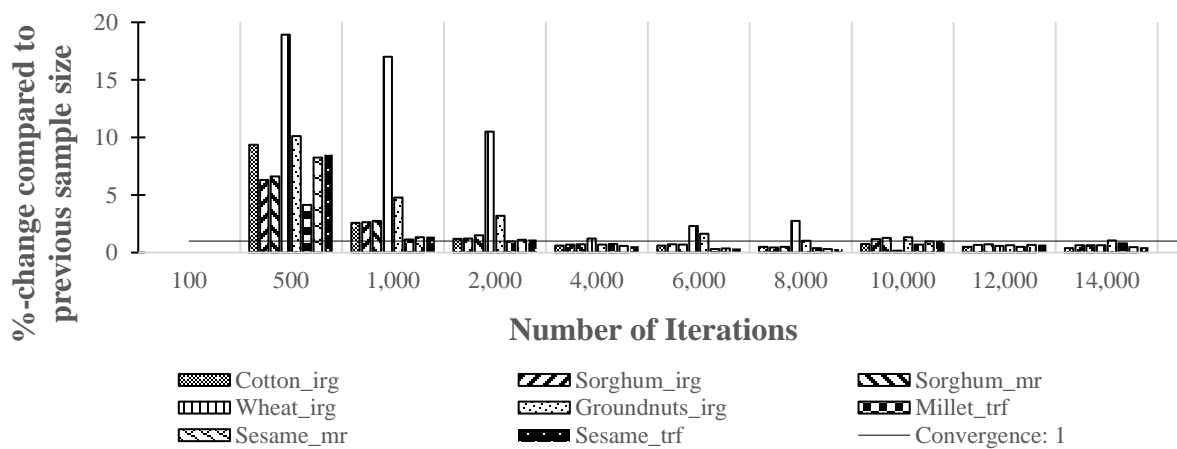
b) GLOBIOM

c) Dynamic CGE

Figure 3. Convergence of the CVs of the prices of the (a) Static CGE and (b) GLOBIOM models and of the average absolute price growth rate over the projected period for the (c) Dynamic CGE model.

Notation: Ind-Indonesia, BR-Brazil, irg-irrigated, mr- mechanized rain-fed, trf- traditional rain-fed.

5.2. MRGQ results

The main advantage of the MRGQ method is that the number of iterations required to achieve robust results is far below the number of iterations necessary for the LHS method. Table 1 presents the number of iterations used by the two methods in each model and the percentage reduction in these numbers by the proposed MRGQ method compared to LHS.

Table 1. Percentage Reduction of Iterations Required by the MRGQ Method Compared to the Converged Sample Size Iterations Required by the LHS Method

	LHS	MRGQ	% reduction
Static CGE	20,000	400	98.0
GLOBIOM	10,000	340	96.6
Dynamic CGE	14,000	280	98.0

While using only a fraction of the iterations required by LHS method, the MRGQ method produces results equal in quality to those delivered by the LHS method and therefore reduces the computational requirements profoundly. Exemplary results from each model are presented in figures 4, 5 and 6 as percent deviations from the benchmark results derived using the LHS method (for the complete results, see Appendix I). These results show two things clearly: First, the dashed bars demonstrate that depending on the rotations of Stroud's octahedron, the generated quadrature points lead to different levels of quality compared to the benchmark results. The largest deviations in the CVs of production and prices from the benchmark presented in figures 4 to 6 are -10% and +10%, respectively, in the Static CGE; +11% and -4%, respectively, in the GLOBIOM model; and -14% and -16%, respectively in the Dynamic CGE. Second, the black lines show that the proposed MRGQ method delivers results very close to the benchmark while keeping the number of required iterations very small compared to those required by the probabilistic methods.
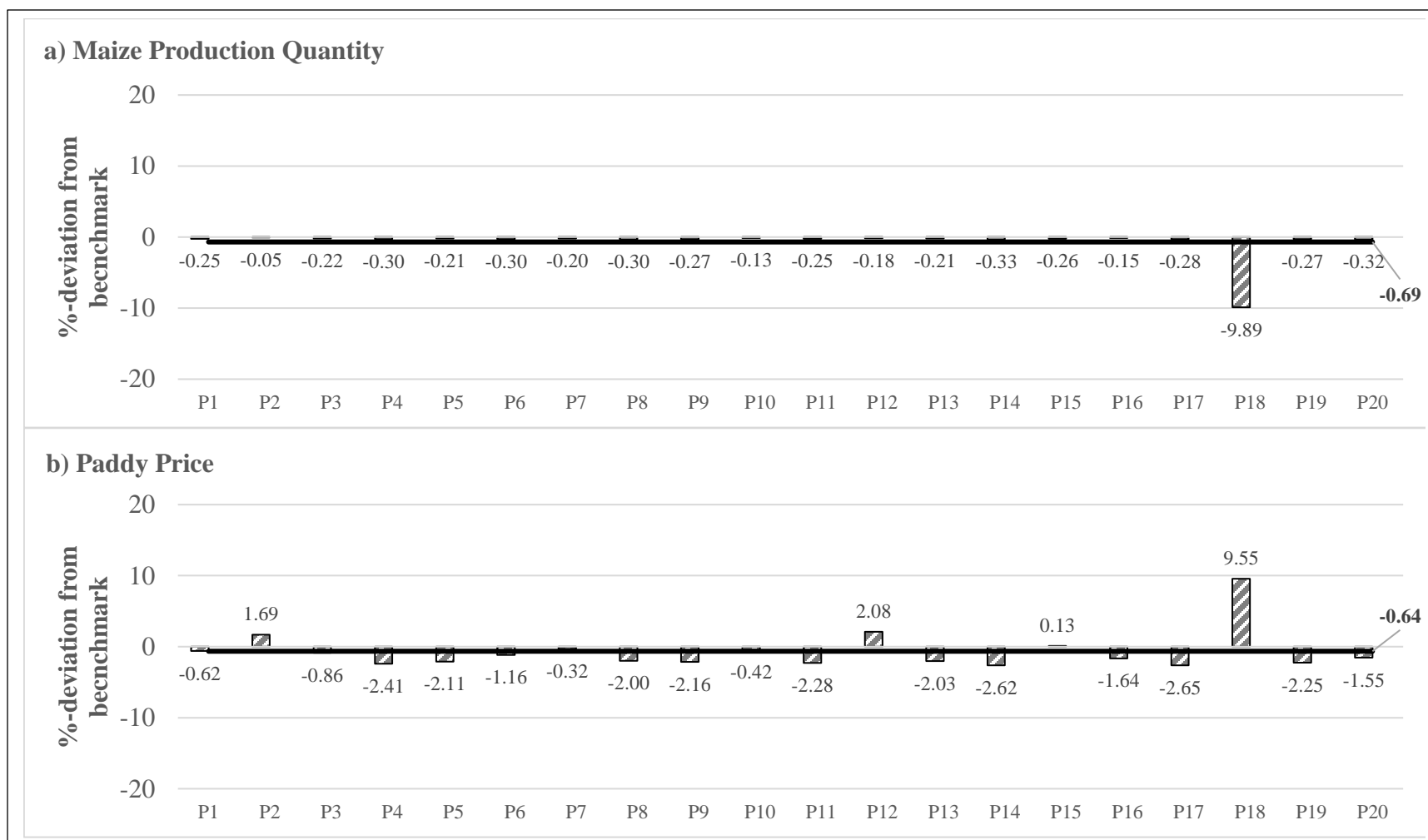
Figure 4. Precision of GQ and MRGQ in the *Static CGE* model measured in percent deviations of the CVs from the benchmark (LHS with 20,000 iterations) for (a) maize production quantities and (b) paddy prices in Bhutan. P1-P20: results by individual rotations; black line: MRGQ results.
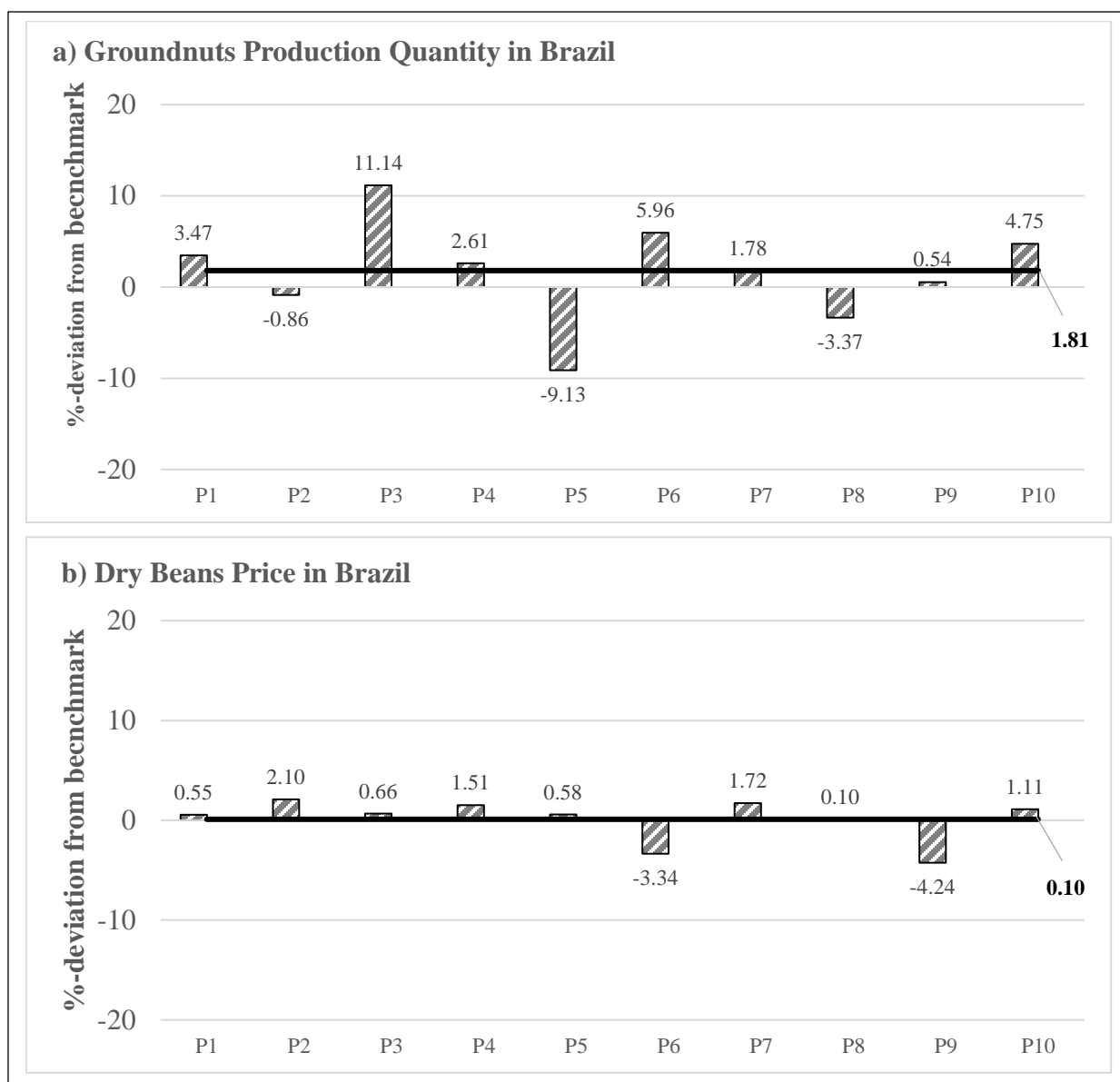
Figure 5. Precision of GQ and MRGQ in the *GLOBIOM* model measured in percent deviations of the CVs from the benchmark (LHS with 10,000 iterations) for (a) groundnuts production quantities and (b) dry beans prices in Brazil. P1-P10: results by individual rotations; black line: MRGQ results.

a) Irrigated Wheat Production Quantity

P1: 7.54, P2: -12.48, P3: 13.34, P4: 0.71, P5: -9.68, P6: 11.57, P7: 2.42, P8: -8.03, P9: 9.47, P10: 13.08, P11: -9.72, P12: -14.12, P13: 9.91, P14: 8.50, P15: -7.00, P16: 13.10, P17: -5.01, P18: -13.63, P19: -7.85, P20: 13.97; MRGQ: 1.06

b) Mechanized Rain-Fed Sesame Price

P1: 5.28, P2: -6.99, P3: 2.62, P4: 4.85, P5: -1.90, P6: 6.58, P7: 3.36, P8: -6.79, P9: 5.90, P10: 1.77, P11: -4.36, P12: -10.53, P13: 1.40, P14: 6.77, P15: -16.22, P16: 7.16, P17: -1.95, P18: -12.57, P19: -7.67, P20: 4.91; MRGQ: -0.01
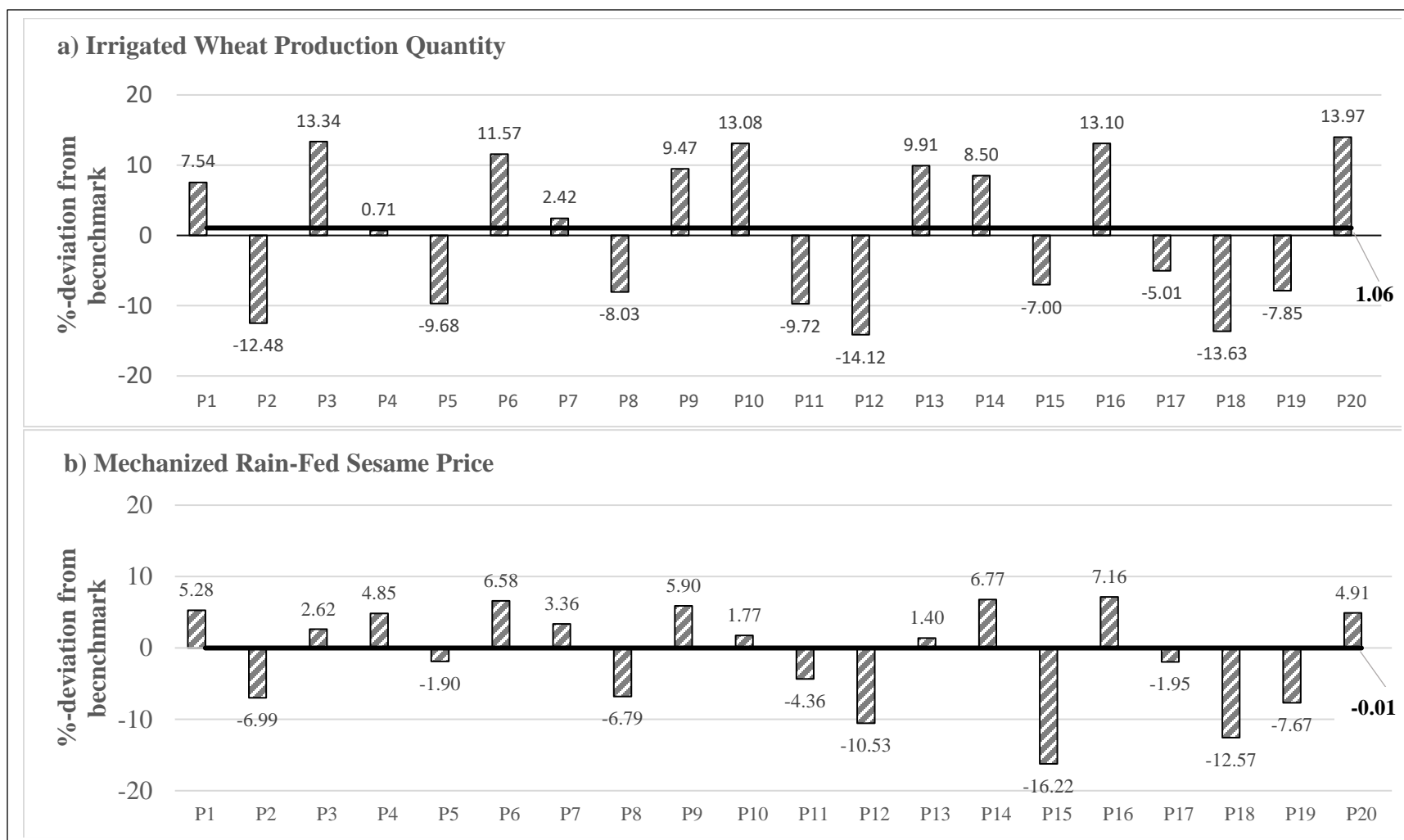
Figure 6. Precision of GQ and MRGQ in the *Dynamic CGE* model. Measured as percent deviations of the CVs of average growth rates from 2021 to 2025 from the benchmark (LHS_14,000) for (a) irrigated wheat production quantities and (b) mechanized rain-fed sesame prices in the Sudan. P1-P20: results by individual rotations; black line: MRGQ results.

In Appendix I, we present the complete results for all stochastic crops in the three models. The difference between the minimum/maximum results and the MRGQ results presented there can be considered a measure for evaluating the model improvements made by the MRGQ method. In all three models, we observe large deviations in the approximated results obtained by a single GQ. More specifically, in the Static CGE, we observe potential inaccuracies ranging from -10% to +1% for production and from -28% to +29% for prices. In GLOBIOM, the inaccuracies range from - 21% to +11% and from -24% to +14% for production and prices, respectively. In the case of the Dynamic CGE, we observe inaccuracies in production within the range of -63% to +20%. The inaccuracies in prices in the Dynamic CGE caused by a single GQ range from -82% to +35% (Appendix I). In the vast majority of cases, we see drastic improvements in the results when applying the MRGQ. The average deviations in the MRGQ results in the Static CGE are +0.04% and -6.00%, in GLOBIOM -0.24% and -1.30% and in the Dynamic CGE +0.09% and +0.90% for production and prices, respectively.

In order to observe the differences between the stochastic shocks produced by both methods and their impacts on the final results, we also analyze their cumulative density functions (CDFs). Figure 7 presents the CDFs of the stochastic shocks generated by the proposed MRGQ method compared to the LHS and of the result-variables from both approaches. The major difference between the shocks generated by those two methods is that unlike the LHS method, MRGQ does not capture the extreme tails of the shocks. However, failing to do so does not affect the accuracy of the approximation of the central moments of the distribution.[6]

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[6] According to two-sample t- and F- tests, the results obtained from the MRGQ and the LHS methods in figure 7 have equal means and variances at the 5 % significance level.
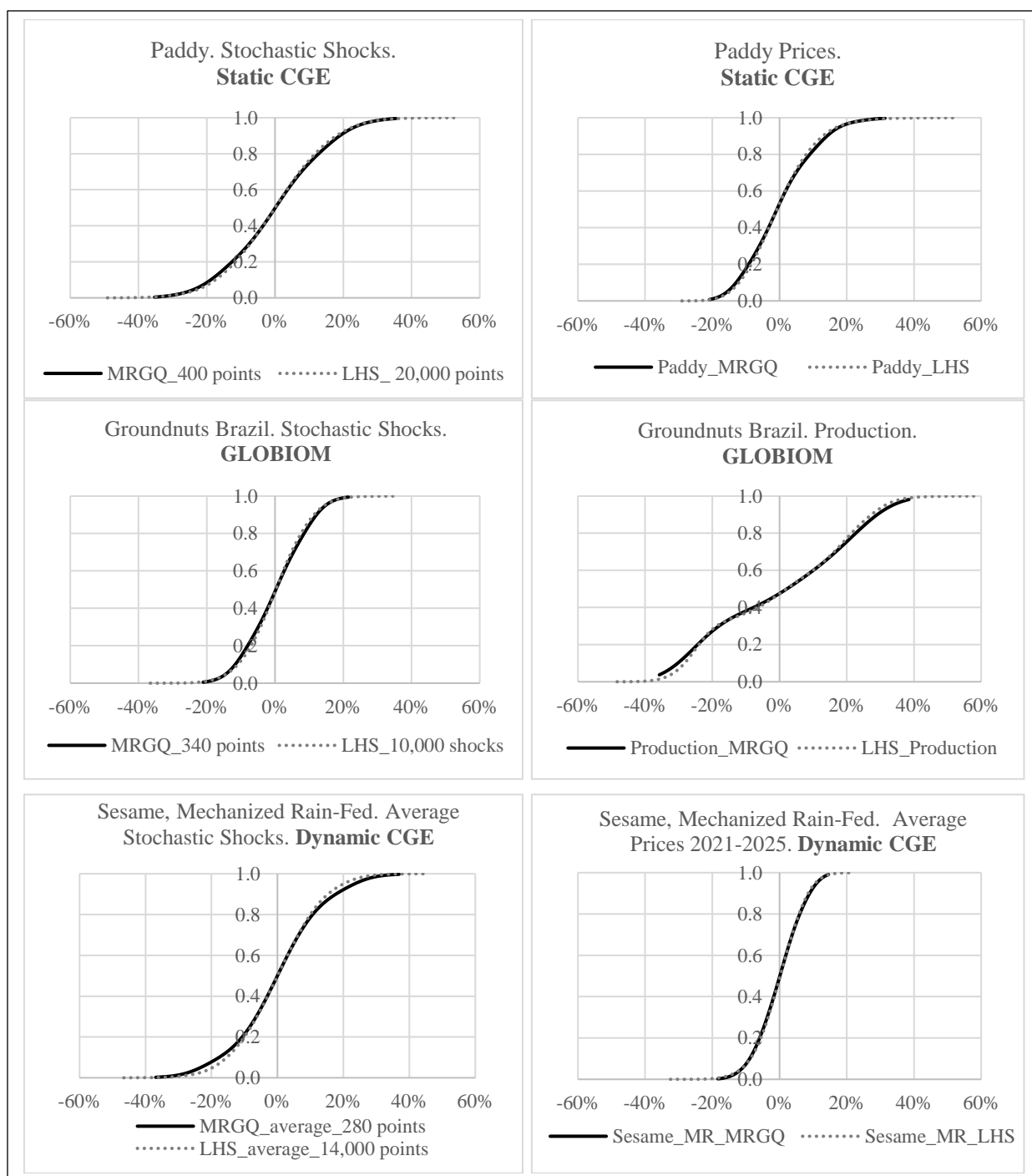
Figure 7. Impact of input uncertainty (left) on output uncertainty (right). Cumulative distribution functions of the stochastic shocks generated by MRGQ and LHS and the percent deviations of the results from the expected values.

Table 2 presents the differences between the LHS method and the proposed novel MRGQ-approach in terms of computational and data management requirements. Due to the modest computational requirements of the Static CGE, we manage to obtain a benchmark with a relatively short solving time and a small results file. Still, solving the same model with the proposed approach (using 240 iterations) is much faster, requiring 8% of the computational time and consuming 3% of the computational space used by LHS.

Out of these three models, GLOBIOM is the most computationally burdensome model to solve using the LHS approach. To solve the GLOBIOM model 10,000 times, 2,500 computer-hours are required. Moreover, the produced results file is very large and none of the available software packages is able to open it. Therefore, we cut it in smaller pieces and analyze them separately. Solving the model with the MRGQ (using only 340 iterations) instead of the LHS approach requires only 3% of both the running time and disk space to produce reliable results. Note that the model is run for one time step only. Each additional time step would increase the requirements multiplicatively.

In the case of the Dynamic CGE, the difficulty arises from its recursive-dynamic setup. The original model is set up to project for the time interval 2018-2050. In order to obtain benchmark results, however, we have to shorten the interval to 2018-2025. Generating a benchmark for a single scenario requires 84 computer-hours of time and, similar to GLOBIOM, Dynamic CGE produces a large results file. In contrast, solving the same model with the MRGQ method (using 280 iterations) requires only 6% of the running time and 9% of the disk space consumed by the LHS method.

Table 2. Computational Requirements of the Multiple Rotations of Gaussian Quadratures and Latin Hypercube Sampling in Three Simulation Models

	LHS		MRGQ			
	Size of results file in GB	Model run time (in computer-hours)	Size of results file in GB	Reduction in the size of results file (percentage reduction from LHS)	Model run time (in computer-hours)	Reduction in model run time (percentage reduction from LHS)
Static CGE	0.9	9	0.03 (20 rotations)	96.7%	0.7	92.2%
GLOBIOM	70.0	2,500	2.36 (10 rotations)	96.6%	160	96.6%
Dynamic CGE	28.0	84	2.60 (20 rotations)	90.7%	5	94.0%

6. Discussion

In this article, we introduce a novel approach to uncertainty analysis targeting large-scale simulation models with computational restrictions. The proposed MRGQ method is based on the degree three quadrature formulae by Stroud (1957) and incorporates a novel approximation error reduction technique which allows computationally burdensome probabilistic approaches to be avoided while reaching an approximation quality comparable to those of such approaches with very large sample sizes.

We test the proposed approach in three simulation models addressing agricultural markets, namely, a comparative static CGE model applied to Bhutan (Static CGE), and a global partial equilibrium model (GLOBIOM) and recursive dynamic CGE model applied to the Sudan (Dynamic CGE). In order to evaluate the accuracy of the results produced by the proposed approach, we generate a benchmark using a probabilistic approach called Latin Hypercube Sampling (LHS) with a converged sample size. To reach convergence, we increase the sample size gradually until the percent deviations of the results compared to those of the previous sample size stay within the interval [-1%, +1%].

We obtain converged results at 14,000, 10,000 and 20,000 iterations for the Static CGE, GLOBIOM and Dynamic CGE models, respectively. These sample sizes are reached by gradually increasing the number of iterations in order to reach the stopping criterion, thus determining the minimum required sample size in each case. For a fair comparison, the resources required to solve the models and analyze the results with smaller sample sizes would actually need to be added to the LHS approach in table 2 because these steps would need to be carried out in order to find the correct sample sizes needed for convergence. Doing so would increase the relative advantages of the MRGQ approach substantially. However, as there is no systematic procedure for determining

the starting number of iterations and the steps for increasing this number, we refrain from doing so here. It is worth noting that most of the studies applying probabilistic approaches to uncertainty analyses in large-scale simulation models hardly ever do any convergence evaluations due to the computational burden. Instead, they often select one sample size that fits the available computational capacities and assume that the produced approximations match the desired quality (e.g., Mary et al. 2018; Valin et al. 2015; Villoria and Preckel 2017), thus underlining the relevance of the MRGQ method: it allows for high-quality stochastic simulations while staying within the usual boundaries of computational capacities.

Depending on the context of the application, there are two potential limitations of the MRGQ method. First, the MRGQ does not capture the extreme tails of distributions. However, the failure to capture the tails can be seen as both a disadvantage and an advantage. On one hand, the inability of MRGQ to depict the outer tails of the distributions, i.e., the effects of extreme shocks, can be viewed as a disadvantage if a researcher is especially interested in studying the impacts of extremes. In this case, we suggest implementing the broader sampling approach via GQ proposed by Preckel et al. (2011) along with the MRGQ method. On the other hand, many simulation models are unable to handle extreme shocks to the system well anyhow, as the systems operate far from their region of calibration and thus the sound empirical foundation of parameters due to technical model constraints. Therefore, when using probabilistic approaches, researchers often truncate the distribution of the shocks anyway (e.g., Hertel et al. 2010; OECD-FAO 2011; Burrell and Nii-naate 2013), which may result in an inaccurate approximation of the central moments of the results. In such a case, MRGQ is the more suitable method for approximating the central moments of the results without losing information about input uncertainty.

The second limitation of the MRGQ method is that it can be applied only to symmetric distributions. In cases of non-symmetric distributions, we suggest extending the MRGQ approach to depict asymmetric regions via the method of DeVuyst and Preckel (2007).

7. Conclusions

This article demonstrates the potential benefits of GQ as an efficient approach to uncertainty analyses in large-scale simulation models but also the limits of traditional GQ approaches, as they may generate approximations of significantly lower quality than those found via traditional probabilistic approaches. We therefore develop and test a novel method, MRGQ. Applying MRGQ in three different simulation models reveals two distinct advantage: First, MRGQ requires a considerably smaller number of iterations to perform an uncertainty analysis compared to the probabilistic approaches. This is especially relevant for large-scale or dynamic simulation models and in cases in which many variables or simulations must be analyzed; second, MRGQ produces highly accurate results with considerably lower computational and data management costs compared to the LHS approach. In light of the usual boundaries to computational capacity, only MRGQ allows to actually conduct a systematic uncertainty analysis with accurate outcomes in large-scale simulation models, as the required sample sizes render probabilistic approaches infeasible. .

The demand for an efficient and robust approach to conduct uncertainty analysis as offered by MRGQ is likely to increase with the ever expanding size and scope of simulation models. Even though computational capacities are growing at a high speed, the computational requirements in times of "big data" will require more efficient methods.

The approach is tested successfully on three very different simulation models, suggesting that it has good potential to be applied as a resource-efficient and highly accurate means of uncertainty

analysis in other large-scale simulation models as well. Thereby, the methodology can be applied for testing the uncertainty of any model parameters, exogenous variables or shocks.

While the successful application of the MRGQ method in three case studies shows its advantages in terms of computational and data management requirements compared to the probabilistic approaches, it also leaves open questions. Future research may generate a better understanding of: a) the optimal number of random rotations required to reach a desired accuracy level given specific model characteristics, and b) the factors affecting the quality of GQ points produced by single rotations of Stroud's octahedron.

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   miss the point%3A stochastic modeling of WTO restrictions&author=P.

   Westhoff&publication_year=2005&pages=87-107.

2. Appendix I

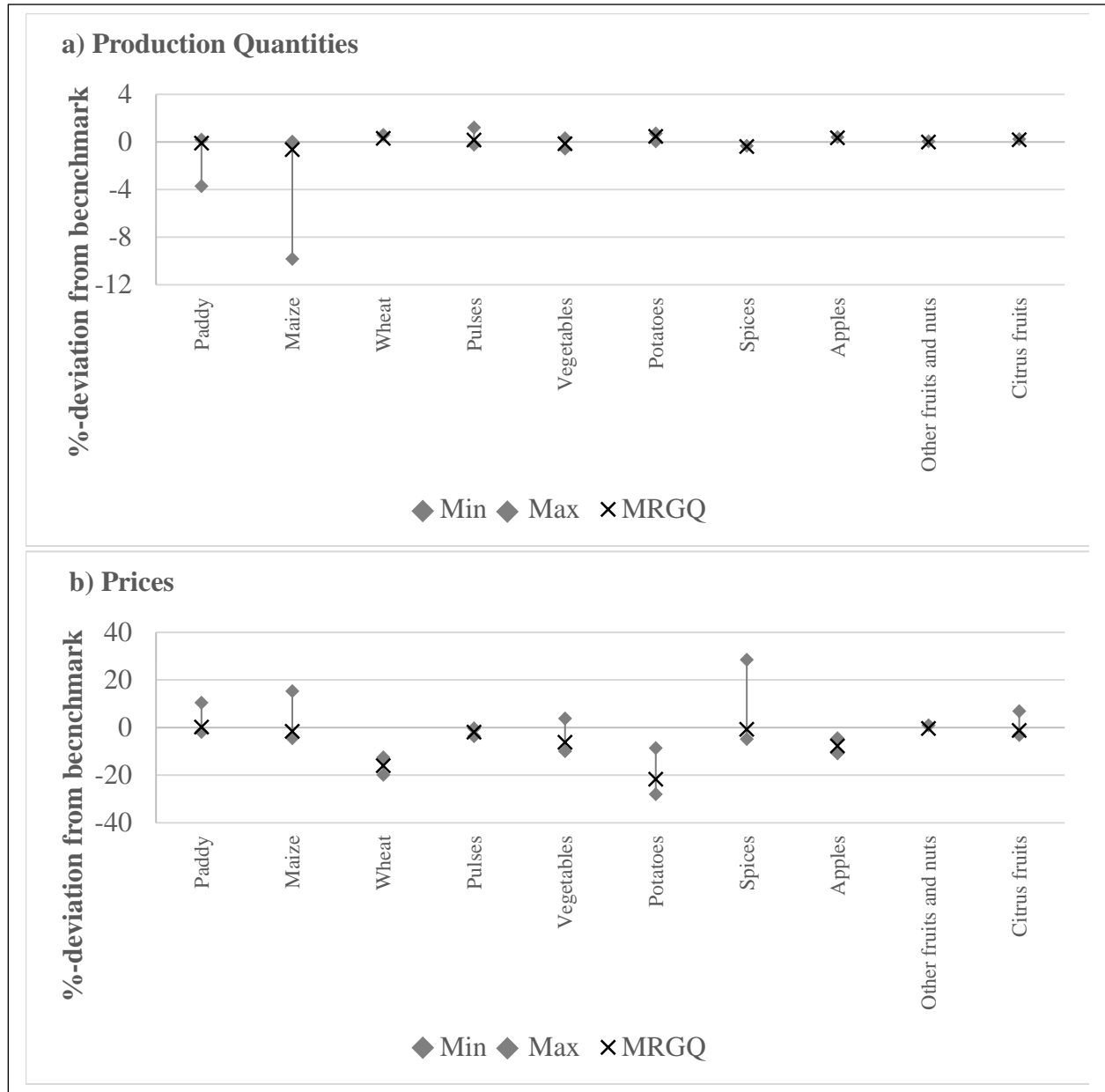**a) Production Quantities**

b) Prices

Figure 9. Range of deviations of results produced by single rotations of GQ in the *Static CGE* model measured in percent deviations of the CVs from the benchmark (LHS with 20,000 iterations). The results obtained by the MRGQ are presented with black crosses.
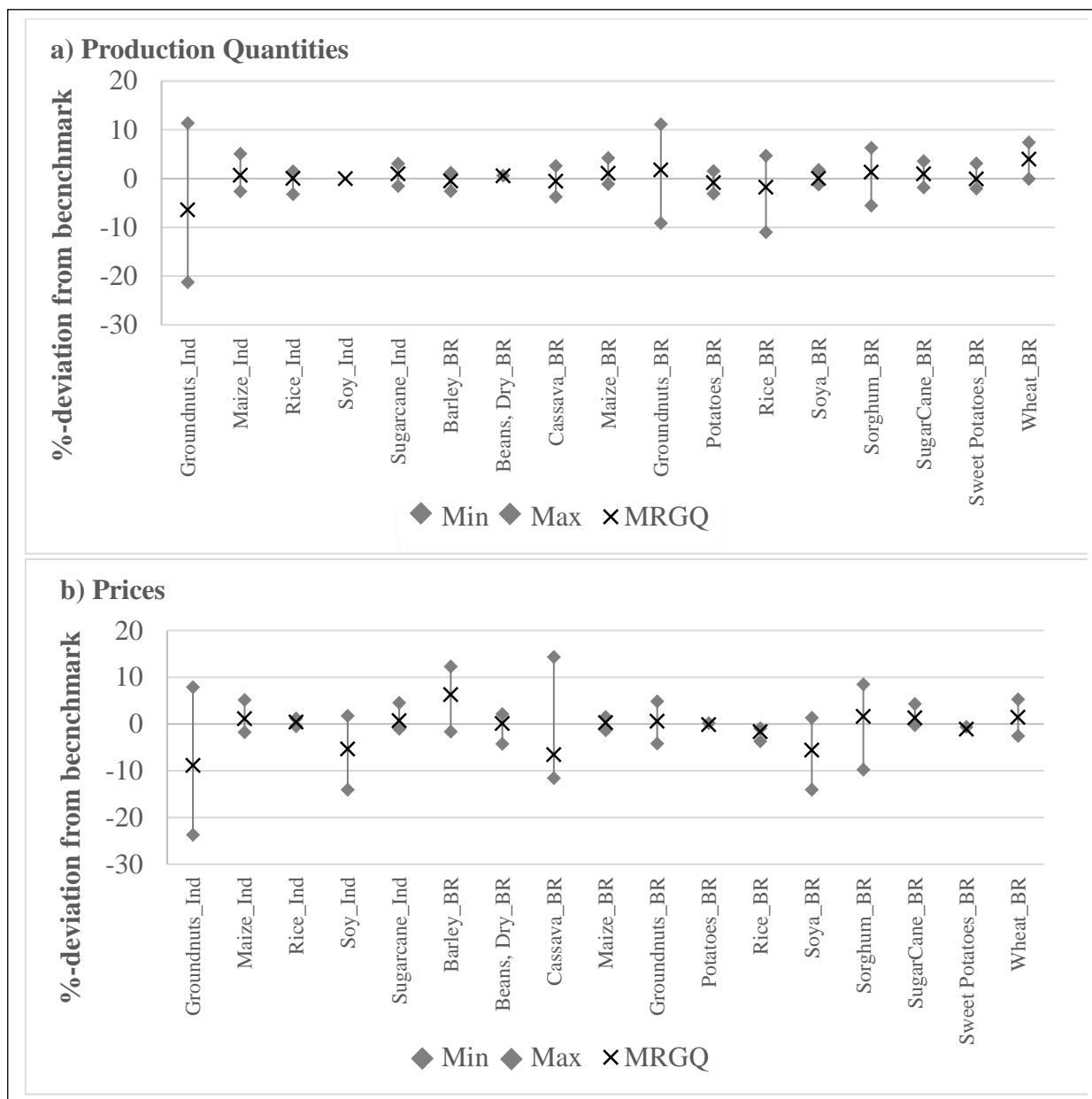
Figure 10. The range of deviations of the results produced by single rotations of GQ in the *GLOBIOM* model measured in percent deviations of the CVs from the benchmark (LHS with 10,000 iterations). The results obtained by the MRGQ are presented with black crosses. Notation: Ind-Indonesia, BR-Brazil.
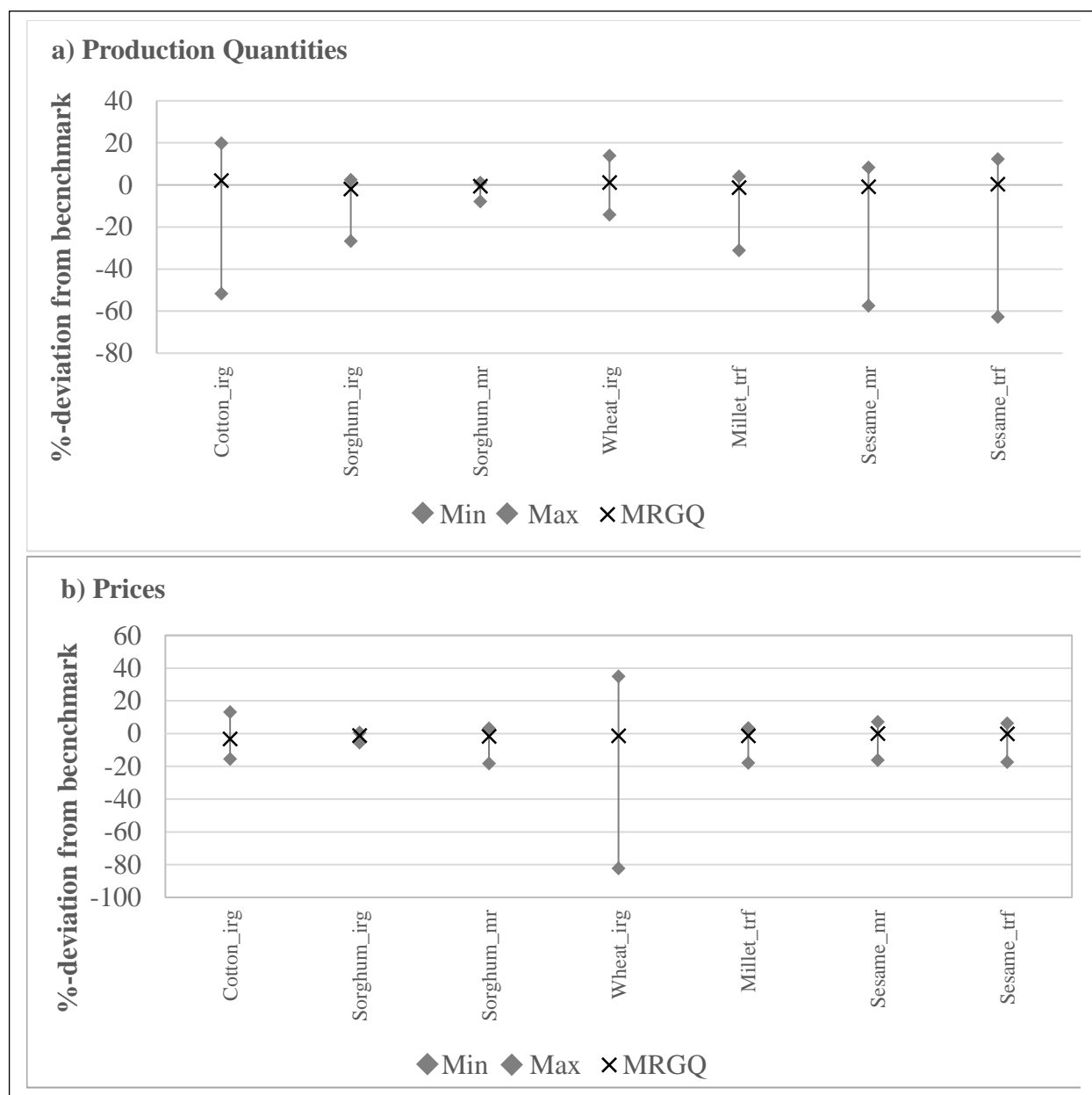
Figure 11. The range of deviations of the results produced by single rotations of GQ in the *Dynamic CGE* model measured in percent deviations of the CVs of average growth rates from the benchmark in the period of 2021 to 2025 from the benchmark (LHS with 14,000 iterations). The results obtained by the MRGQ are presented with black crosses. Notation: irg-irrigated, mr- mechanized rain-fed, trf- traditional rain-fed.