



# Stochastic Simulation with Informed Rotations of Gaussian Quadratures

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Faculty of Life Sciences

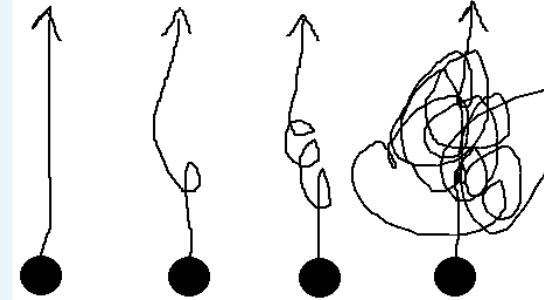
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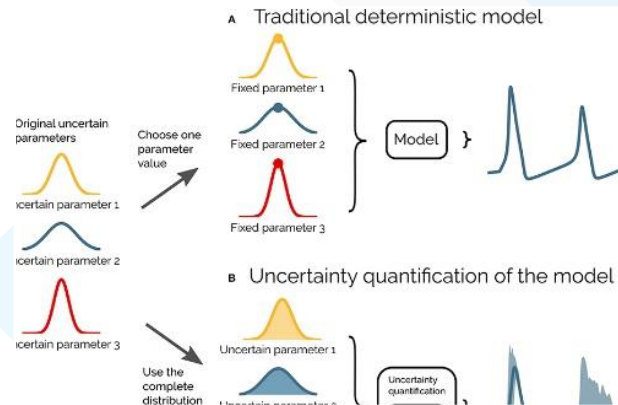
# UA is becoming a good modeling practice



Increase in computational power



Expansion of simulation models in detail and complexity



SSA/UA becoming a standard/good modeling practice



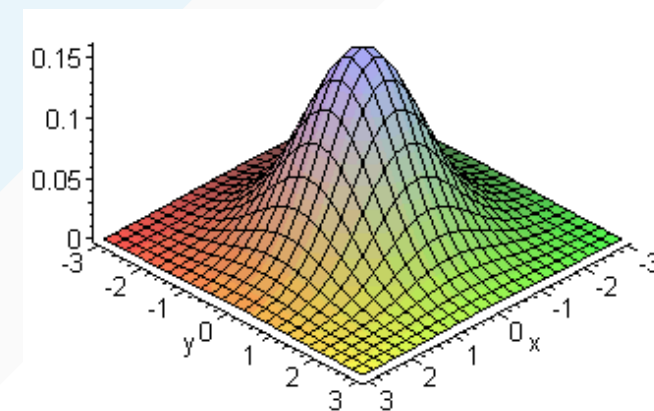
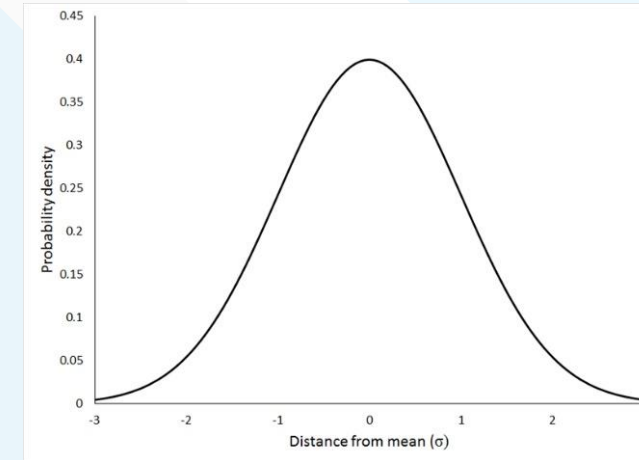
Increased uncertainty associated with model results

# Why is UA a numerical integration problem?

- 1 Model variable/parameter:  $x$  (e.g., yields, prices, elasticities, etc.)
- 2 Pdf describing the uncertainty around  $x$ :  $g(x)$
- 3 Model function:  $f(x)$

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

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



# Categorization of the methods according to Haber (1970)

## Probabilistic

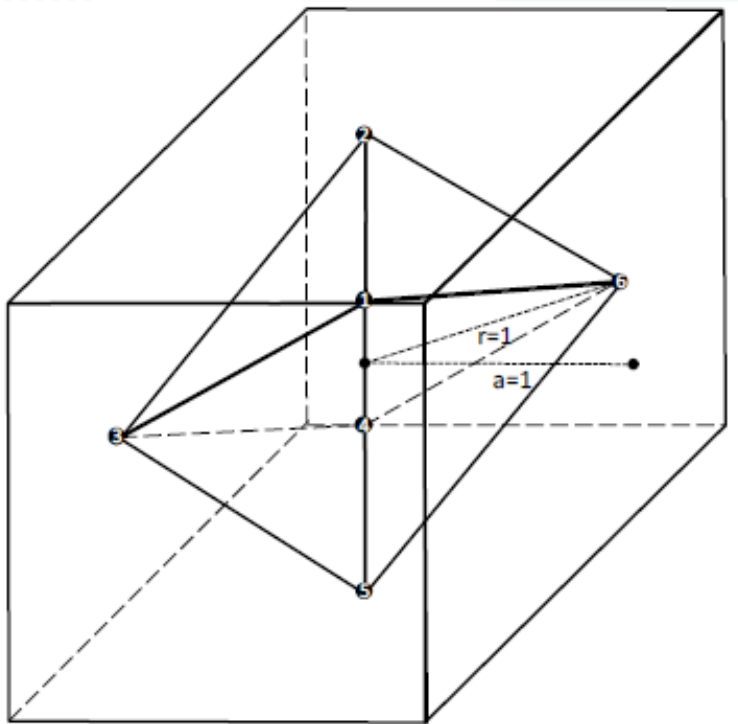
- 1 Monte Carlo (MC) (Metropolis and Ulam 1949)
- 2 Stratified sampling (e.g., Saltelli et al. 2008; Norton 2015)
- 3 Latin hypercube sampling (LHS) (Helton and Davis 2003)

**Convergence evaluation**

## Efficient

- 1 Gaussian quadratures
  - Degree 3 quadrature formulae by Stroud (1957)

# Stroud's (1957) theorem for degree 3 quadrature formulae



Source: Artavia et al. (2015)

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

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

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

For  $k = 1, \dots, 2n,$

$$j = 1, \dots, \left\lfloor \frac{n}{2} \right\rfloor$$

# Categorization of the methods according to Haber (1970)

## Probabilistic

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**Convergence evaluation**

## Efficient

- 1 Gaussian quadratures
  - Degree 3 quadrature formulae by Stroud (1957)
  - Arndt (1996) adapted Stroud's formulae for integrals with MSND as a weight function

$$GQ = A\Gamma + \vec{\mu} [1 \dots 1]$$



$$\Sigma = AA^T \quad \Gamma_k = (\gamma_{k,1}, \gamma_{k,2}, \dots, \gamma_{k,n})$$

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

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

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

# Current state of art

Arndt (1996)

Introduced Stroud's (1957) order 3 GQ in the GTAP model.

Preckel et al. (2011a)

Research question:

The impact of limited sampling interval of the GQ method.

Finding:

Sampling breadth is important for highly nonlinear models.

Preckel et al. (2011b)

Research question:

The impact of using different linear transformation methods.

Finding:

Noncrucial for the quality of the results.

Artavia et al. (2015)

Research question:

Do rotations of Stroud's octahedron matter?

Finding:

Yes, they do!

Villoria and Preckel (2017)

Research question:

Evaluating the quality of GQ results compared to MC results.

Finding:

Large differences in the first three moments of the pdfs of the results.



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# Environmental Modelling and Software

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## Multiple rotations of Gaussian quadratures: An efficient method for uncertainty analyses in large-scale simulation models

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### ARTICLE INFO

#### Keywords:

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Systematic sensitivity analysis  
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Multiple rotations of Gaussian quadratures  
Monte Carlo sampling  
Computable general equilibrium models  
Partial equilibrium models

### ABSTRACT

Concerns regarding the impact of climate change, food price volatility, and weather uncertainty have motivated users of simulation models to consider uncertainty in their simulations. One way to do this is to integrate uncertainty components in the model equations, thus turning the model into a problem of numerical integration. Most of these problems do not have analytical solutions, and researchers, therefore, apply numerical approximation methods. This article presents a novel approach to conducting an uncertainty analysis as an alternative to the computationally burdensome Monte Carlo-based (MC) methods. The developed method is based on the degree three Gaussian quadrature (GQ) formulae and is tested using three large-scale simulation models. While the standard single GQ method often produces low-quality approximations, the results of this study demonstrate that the proposed approach reduces the approximation errors by a factor of nine using only 3.4% of the computational effort required by the MC-based methods in the most computationally demanding model.



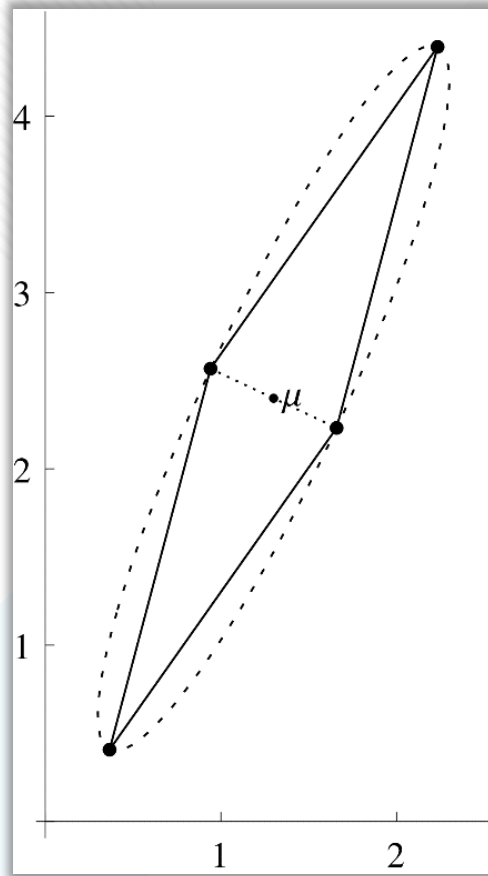
# Identification of good rotations

- **Campolongo et al. (2007)**
  - Improving the EE method (Morris 1991) by maximizing the dispersion of the sampling points in the input space.
- **Dispersion of a GQ family**

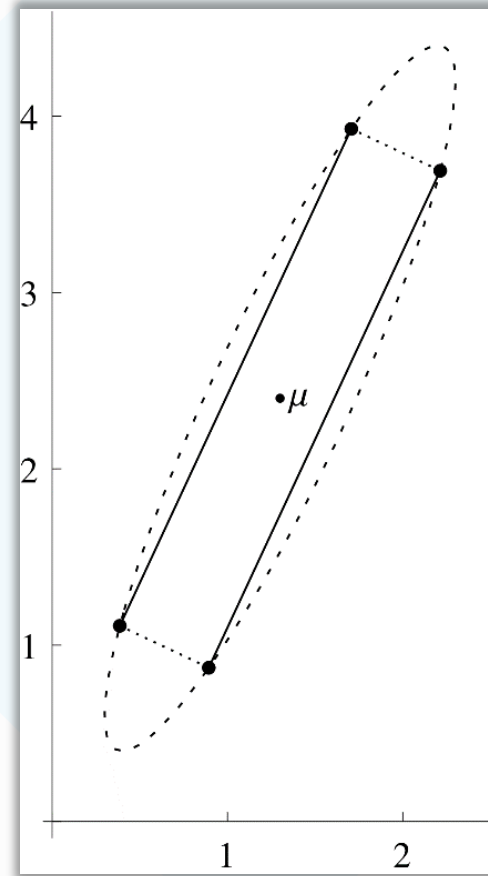
$$\text{disp}(\overrightarrow{GQ_k}) = \min_{j \neq i} \|x_j - x_i\|$$

$$\max(\text{disp}(\overrightarrow{GQ_k}))$$

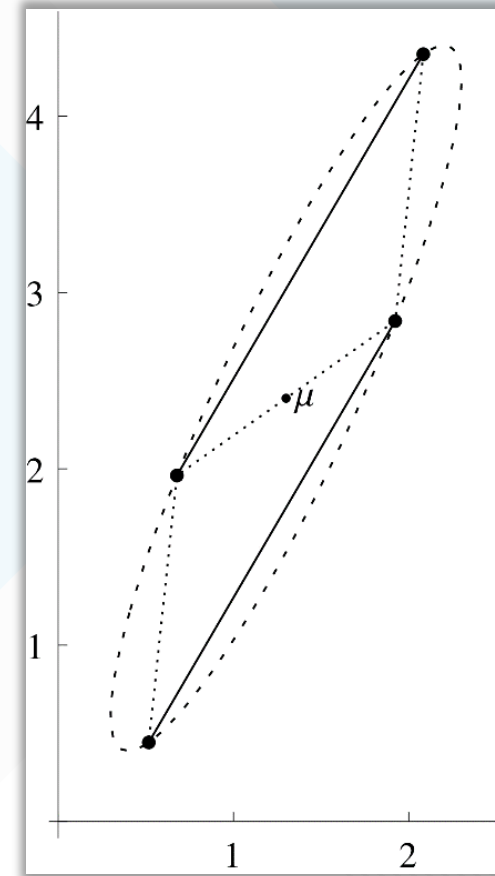
# The IRGQ method in R2



(a)

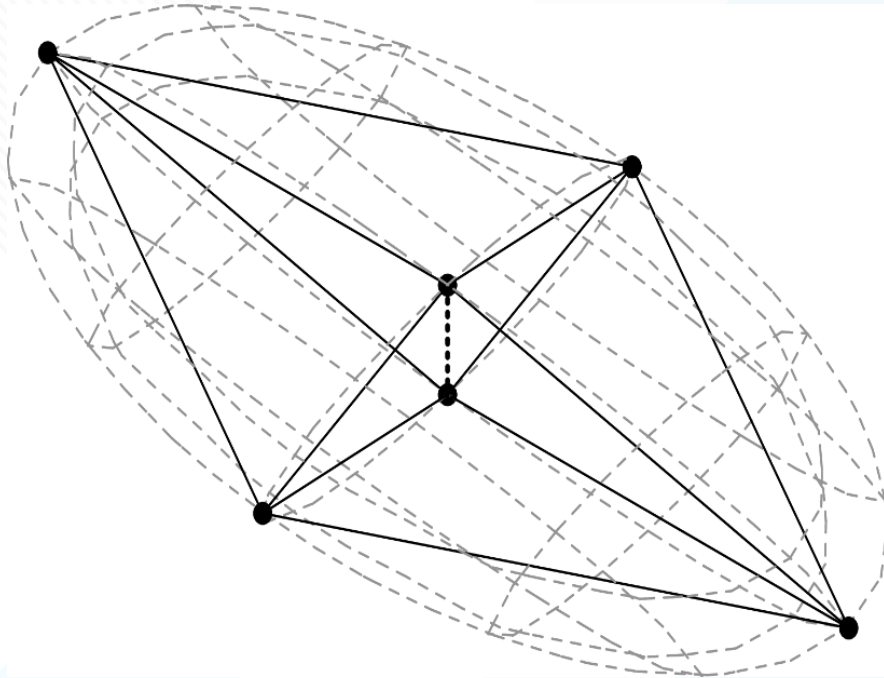


(b)

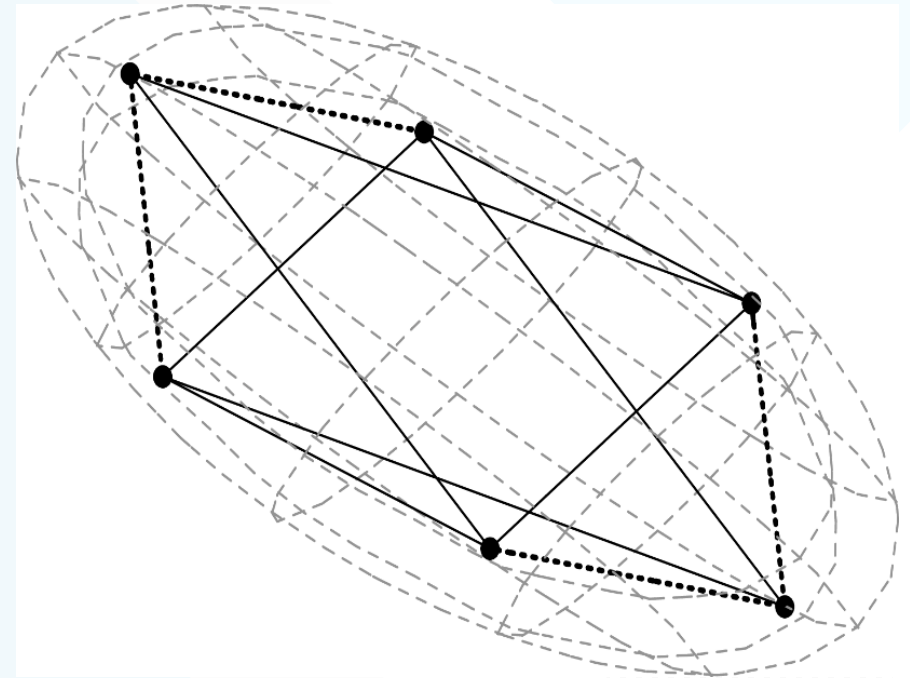


(c)

# The IRGQ method in R3



(a)



(b)

# Simulation models used

## ESIM

- Partial equilibrium (PE) (Grethe 2012)
- GLOBAL (16 regional groups, 3 crops)
- 42 stochastic variables
- Benchmarks by (Artavia et al. 2015)

## GLOBIOM

- Partial equilibrium (PE) (Havlík et al. 2011; Havlík et al. 2014)
- Bottom-up
- Recursive-dynamic
- Global (31 regions, 18 crops)

## Dynamic CGE

- Single-country
- Recursive-dynamic CGE model (Diao and Thurlow 2012)
- linked to the IMPACT modeling system (Robinson et al. 2015)
- 2012 SAM for the Sudan (Siddig et al. 2018)

# Experimental design

- 10 rotations with maximal dispersion for each model
- 10 rotations with minimal dispersion for each model
- Compare with benchmarks obtained by LHS
- Analyzing yield uncertainty

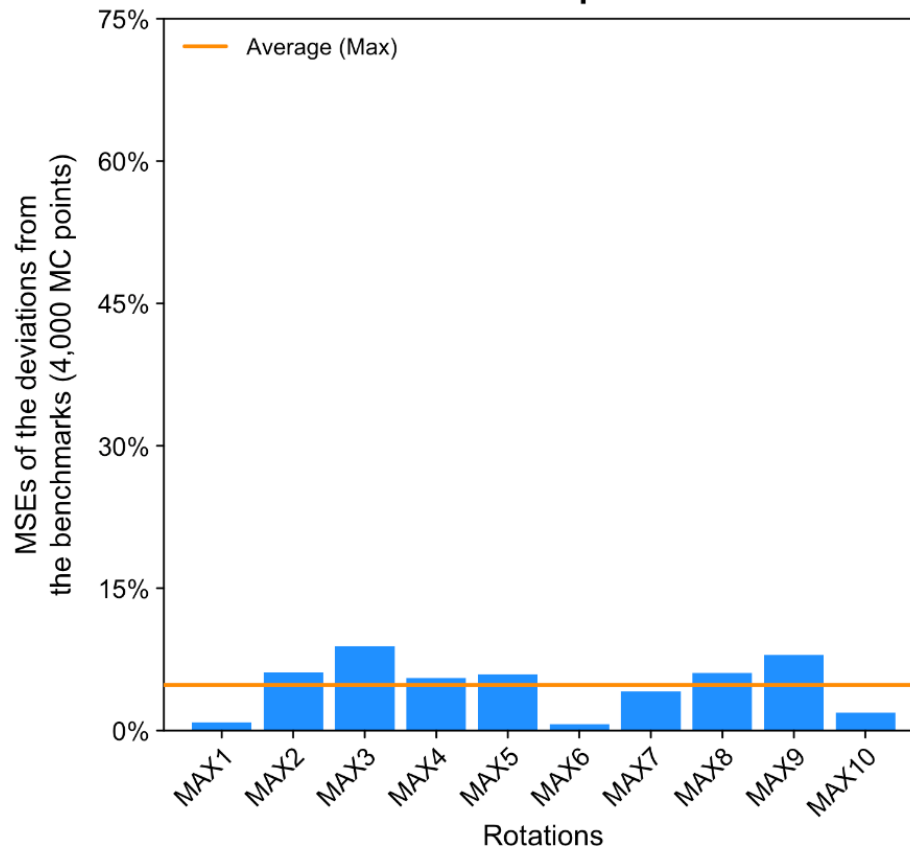


# Percentage deviations of the CVs of producer prices in the “ROW” from the benchmarks. ESIM

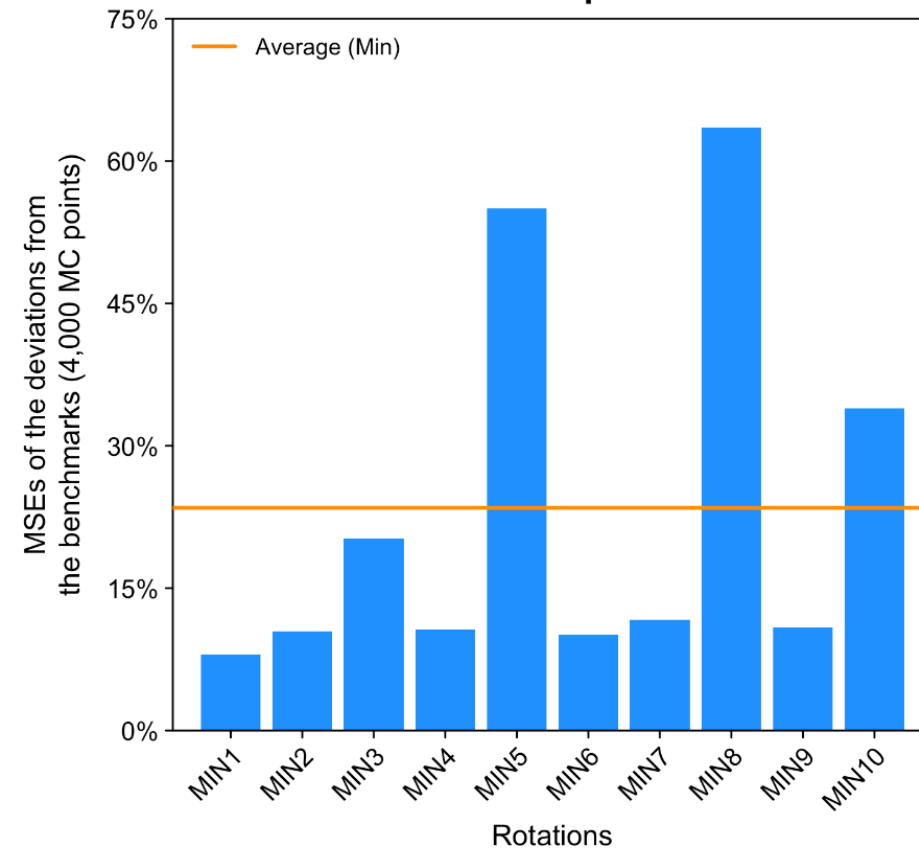
| Results obtained by the GQs with maximal dispersion |        |          |        |       | Results obtained by the GQs with minimal dispersion |        |          |        |        |
|-----------------------------------------------------|--------|----------|--------|-------|-----------------------------------------------------|--------|----------|--------|--------|
|                                                     | Barley | Rapeseed | Wheat  | MSE   |                                                     | Barley | Rapeseed | Wheat  | MSE    |
| MAX1                                                | 1.388  | 0.133    | -0.799 | 0.861 | MIN1                                                | 3.672  | 2.832    | -1.627 | 8.050  |
| MAX2                                                | -3.340 | 0.405    | -2.654 | 6.120 | MIN2                                                | -3.508 | 0.790    | -4.305 | 10.490 |
| MAX3                                                | -4.052 | 0.855    | -3.103 | 8.928 | MIN3                                                | -3.885 | 0.161    | -6.760 | 20.272 |
| MAX4                                                | 2.058  | 1.523    | 3.163  | 5.520 | MIN4                                                | -5.283 | 0.414    | -1.956 | 10.637 |
| MAX5                                                | -3.573 | 0.806    | -2.097 | 5.938 | MIN5                                                | -9.431 | 1.245    | -8.638 | 55.034 |
| MAX6                                                | 1.109  | 0.811    | -0.262 | 0.652 | MIN6                                                | 5.387  | 0.931    | 0.685  | 10.117 |
| MAX7                                                | -3.416 | 0.745    | -0.310 | 4.107 | MIN7                                                | -5.034 | 1.592    | 2.686  | 11.695 |
| MAX8                                                | -3.773 | 0.069    | -1.987 | 6.064 | MIN8                                                | 13.512 | 0.582    | -2.776 | 63.539 |
| MAX9                                                | -3.909 | 0.035    | -2.937 | 7.970 | MIN9                                                | -4.608 | -0.572   | -3.337 | 10.899 |
| MAX10                                               | 0.183  | 0.818    | -2.245 | 1.914 | MIN10                                               | -5.607 | -2.424   | -8.037 | 33.972 |

# ESIM. Results obtained by GQs with max dispersion vs. min dispersion

CVs of the producer prices in the rest of the world.  
Maximal dispersion

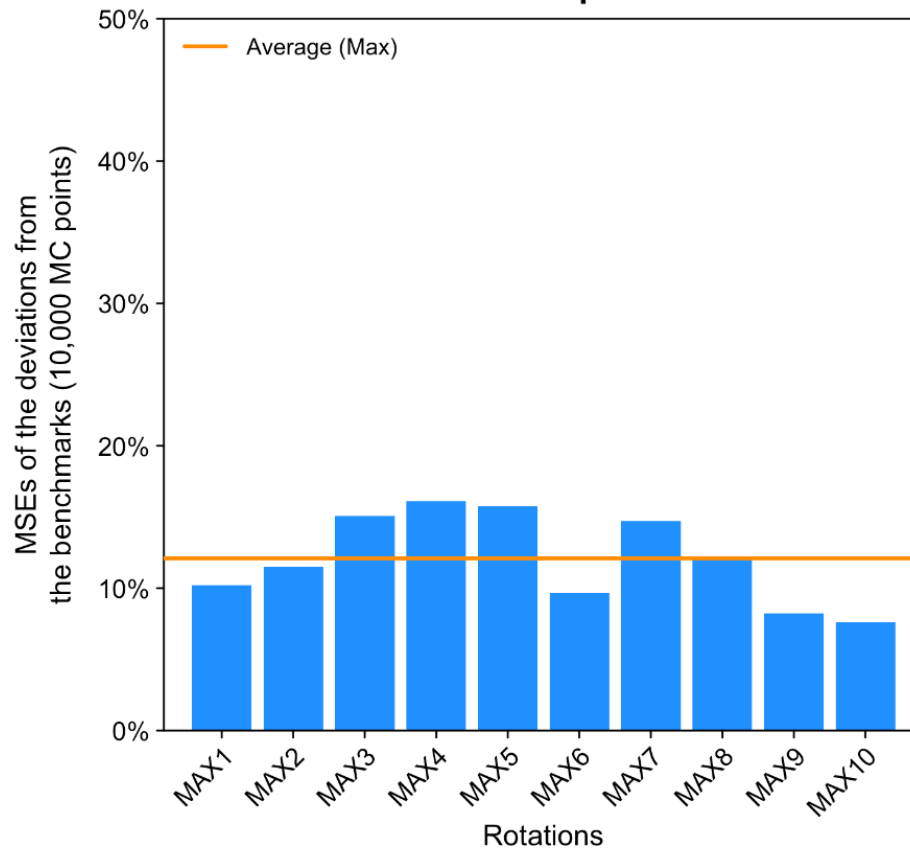


CVs of the producer prices in the rest of the world.  
Minimal dispersion

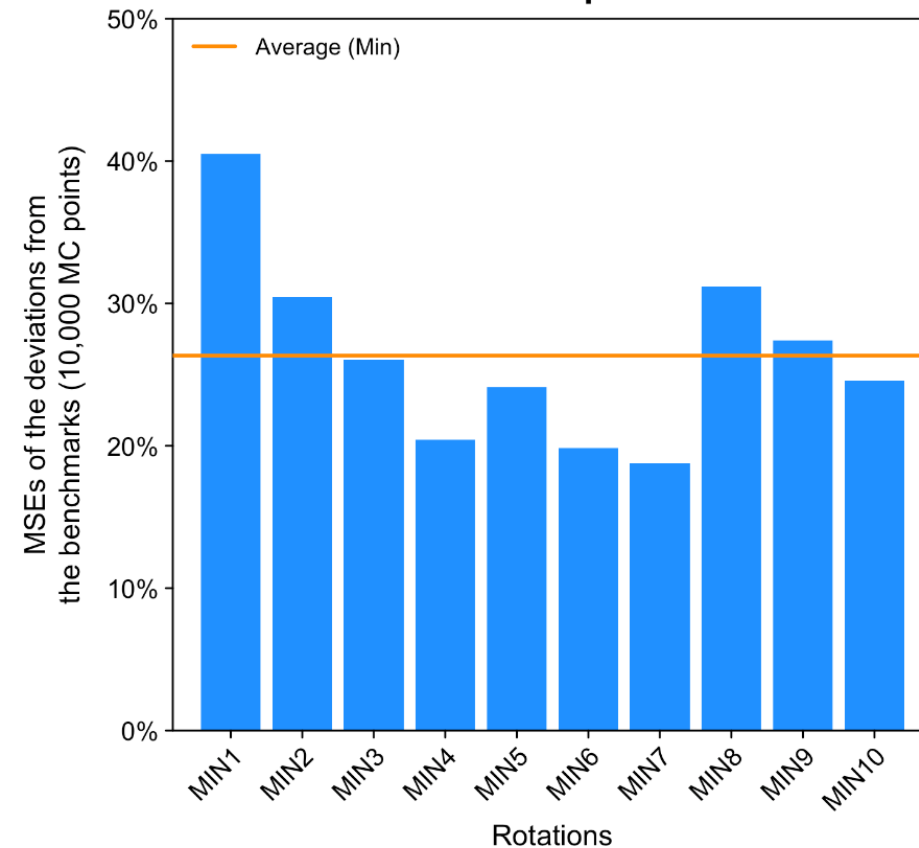


# GLOBIOM. Results obtained by GQs with max dispersion vs. min dispersion

CVs of production quantities in Indonesia and Brazil.  
Maximal dispersion

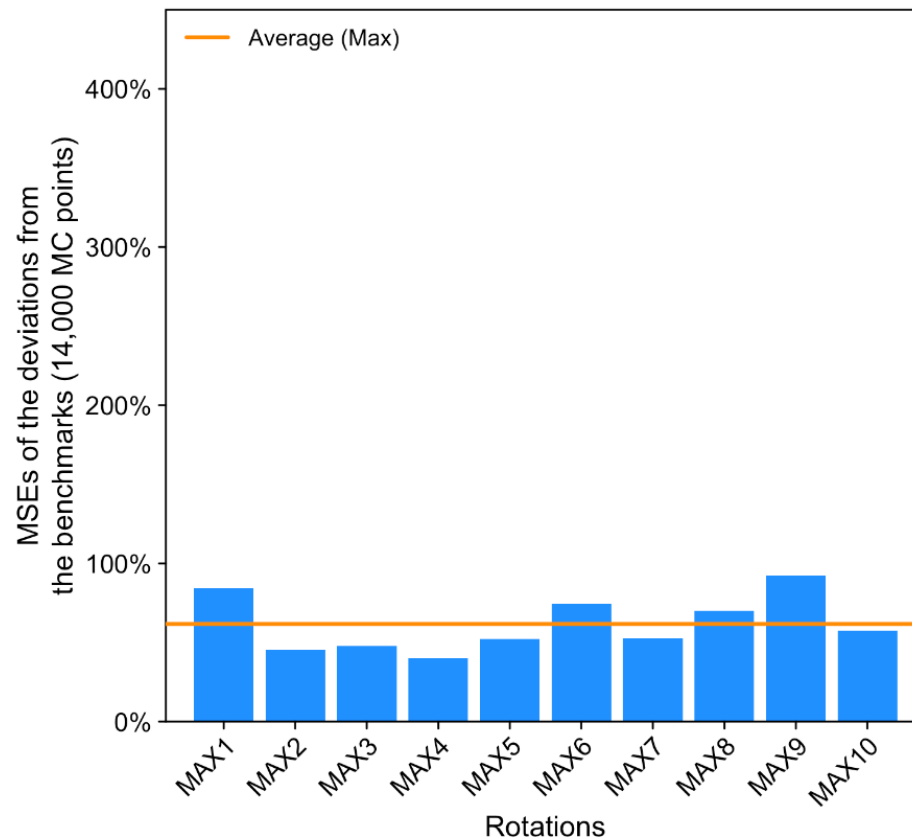


CVs of production quantities in Indonesia and Brazil.  
Minimal dispersion

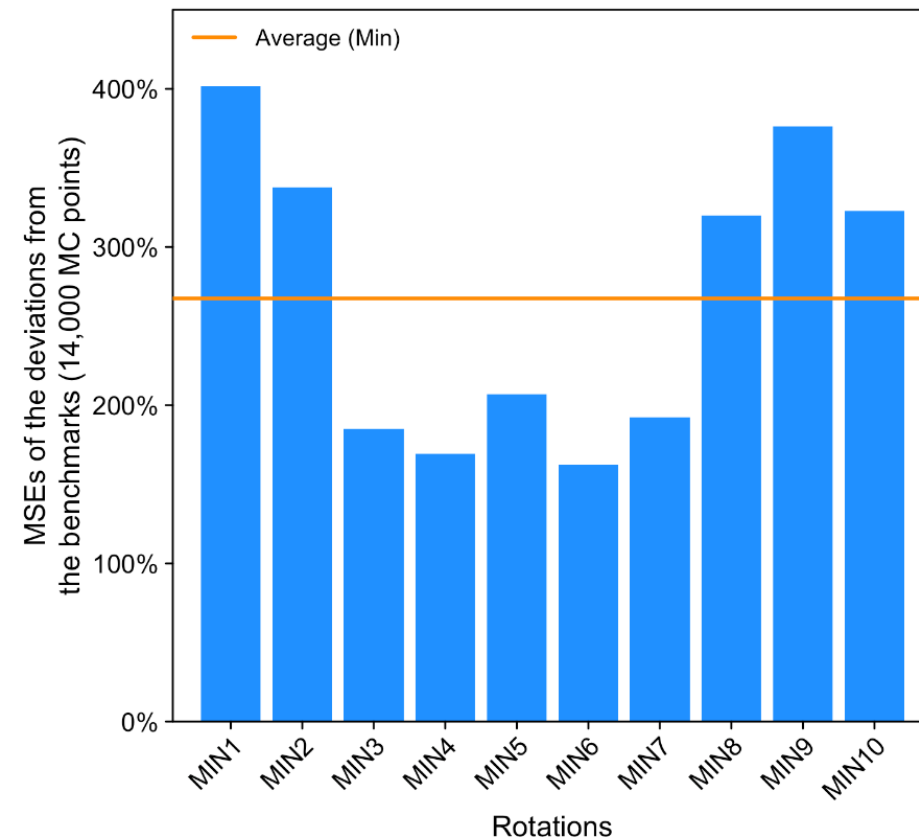


# Dynamic CGE. Results obtained by GQs with max dispersion vs. min dispersion

CVs of production quantities in the Sudan.  
Maximal dispersion



CVs of production quantities in the Sudan.  
Minimal dispersion



# Discussion

## Limitations of the IRGQ method

- Extreme tails of the distributions are not captured
  - **Disadvantage:** if studying the impacts of extremes
    - Implement IRGQ along with Preckel's et al. (2011a) broader sampling approach
  - **Advantage:** many models are unable to handle large shocks
    - Truncate the distribution of shocks vs. IRGQ
- Restricted to approximating symmetric distributions
  - The central idea can be applied to other distributions

# Future research agenda

- **Testing the proposed approaches to**
  - Widening the sampling intervals
  - Extending the methods to depict asymmetric distribution
- **Exploring other factors influencing the quality of the GQ method**
- **Reducing the dimensionality of the problem**
- **Applying and testing the proposed methods in other simulation models addressing policy-relevant questions**



THANK YOU



# References

- Arndt, C. (1996): An Introduction to Systematic Sensitivity Analysis via Gaussian Quadrature. GTAP Technical Paper (2). Available online at <https://docs.lib.purdue.edu/cgi/viewcontent.cgi?referer=&httpsredir=1&article=1002&context=gtatp>.
- Artavia, M.; Grethe, H.; Zimmermann, G. (2015): Stochastic market modeling with Gaussian Quadratures: Do rotations of Stroud's octahedron matter? In *Economic Modelling* 45, pp. 155–168. DOI: 10.1016/j.econmod.2014.10.017.
- Campolongo, F.; Cariboni, J.; Saltelli, A. (2007): An effective screening design for sensitivity analysis of large models. In *Environmental Modelling & Software* 22 (10), pp. 1509–1518. DOI: 10.1016/j.envsoft.2006.10.004.
- Diao, X.; Thurlow, J. (2012): A recursive dynamic computable general equilibrium model. In X. Diao, J. Thurlow, S. Benin, S. Fan (Eds.): *Strategies and priorities for African agriculture. Economywide perspectives from country studies*. Washington, D.C.: International Food Policy Research Institute (IFPRI). DOI: 10.2499/9780896291959.
- Grethe, H. (ed.) (2012): *European Simulation Model (ESIM): Documentation (Model Code, Parameterization, Database)*. Available online at <https://apo.uni-hohenheim.de/en/organization/publication/european-simulation-model-esim-documentation-model-code-parameterization-database-version-of-december-11-2012>.
- Havlík, P.; Schneider, U. A.; Schmid, E.; Böttcher, H.; Fritz, S.; Skalský, R. et al. (2011): Global land-use implications of first and second generation biofuel targets. In *Energy Policy* 39 (10), pp. 5690–5702. DOI: 10.1016/j.enpol.2010.03.030.
- Havlík, P.; Valin, H.; Herrero, M.; Obersteiner, M.; Schmid, E.; Rufino, M. C. et al. (2014): Climate change mitigation through livestock system transitions. In *Proceedings of the National Academy of Sciences of the United States of America* 111 (10), pp. 3709–3714. DOI: 10.1073/pnas.1308044111.
- Helton, J. C.; Davis, F. J. (2003): Latin hypercube sampling and the propagation of uncertainty in analyses of complex systems. In *Reliability Engineering & System Safety* 81 (1), pp. 23–69. DOI: 10.1016/S0951-8320(03)00058-9.
- Metropolis, N.; Ulam, S. (1949): The Monte Carlo method. In *Journal of the American Statistical Association* 44 (247), pp. 335–341. DOI: 10.2307/2280232.

# References

- Morris, M. D. (1991): Factorial Sampling Plans for Preliminary Computational Experiments. In *Technometrics* 33 (2), pp. 161–174. DOI: 10.2307/1269043.
- Norton, J. (2015): An introduction to sensitivity assessment of simulation models. In *Environmental Modelling & Software* 69, pp. 166–174. DOI: 10.1016/j.envsoft.2015.03.020.
- Preckel, P. V.; Verma, M.; Hertel, T.; Martin, W. (2011a): Implications of Broader Sampling Strategy in the Contest of the Special Safeguard Mechanism. In : Presented at the 14th Annual Conference on Global Economic Analysis, Venice, Italy. Global Trade Analysis Project (GTAP). Department of Agricultural Economics, Purdue University, West Lafayette, IN. Available online at [https://www.gtap.agecon.purdue.edu/resources/res\\_display.asp?RecordID=3570](https://www.gtap.agecon.purdue.edu/resources/res_display.asp?RecordID=3570).
- Preckel, P. V.; Verma, M.; Hertel, T.; Martin, W. (2011b): Systematic Sensitivity Analysis for GTAP – Where We’ve Been and Where We’re Going. In : Presented at the 14th Annual Conference on Global Economic Analysis, Venice, Italy. Global Trade Analysis Project (GTAP). Department of Agricultural Economics, Purdue University, West Lafayette, IN. Available online at [https://www.gtap.agecon.purdue.edu/resources/res\\_display.asp?RecordID=3565](https://www.gtap.agecon.purdue.edu/resources/res_display.asp?RecordID=3565).
- Robinson, S.; Mason-D’Croz, D.; Islam, S.; Sulser, T. B.; Robertson, R.; Zhu, T. et al. (2015): The International Model for Policy Analysis of Agricultural Commodities and Trade (IMPACT). Model Description for Version 3. International Food Policy Research Institute (IFPRI). Washington, D.C. Available online at <http://ebrary.ifpri.org/cdm/ref/collection/p15738coll2/id/129825>.
- Saltelli, A.; Ratto, M.; Andres, T.; Campolongo, F.; Cariboni, J.; Gatelli, D. et al. (2008): *Global sensitivity analysis: The primer*. John Wiley & Sons, Ltd, Chichester, West Sussex.
- Siddig, Khalid; Stepanyan, Davit; Wiebelt, Manfred; Grethe, Harald; Zhu, Tingju (2020): Climate change and agriculture in the Sudan: Impact pathways beyond changes in mean rainfall and temperature. In *Ecological Economics* 169, p. 106566. DOI: 10.1016/j.ecolecon.2019.106566.
- Stepanyan, Davit; Grethe, Harald; Zimmermann, Georg; Siddig, Khalid; Deppermann, Andre; Feuerbacher, Arndt; Luckmann, Jonas; Valin, Hugo; Nishizawa, Takamasa; Ermolieva, Tatiana; Havlik, Petr (2021): Multiple rotations of Gaussian quadratures: an efficient method for uncertainty analyses in large-scale simulation models. In *Environmental Modelling & Software*, 136. DOI: 10.1016/j.envsoft.2020.104929.

# References

- Stroud, A. H. (1957): Remarks on the Disposition of Points in Numerical Integration Formulas. In Mathematical Tables and Other Aids to Computation 11 (60), pp. 257–261. Available online at [https://www.jstor.org/stable/2001945?seq=1#metadata\\_info\\_tab\\_contents](https://www.jstor.org/stable/2001945?seq=1#metadata_info_tab_contents).
- Villoria, N. B.; Preckel, P. V. (2017): Gaussian Quadratures vs. Monte Carlo Experiments for Systematic Sensitivity Analysis of Computable General Equilibrium Model Results. In Economics Bulletin 37 (1), pp. 480–487. Available online at <http://www.accessecon.com/Pubs/EB/2017/Volume37/EB-17-V37-I1-P43.pdf>.



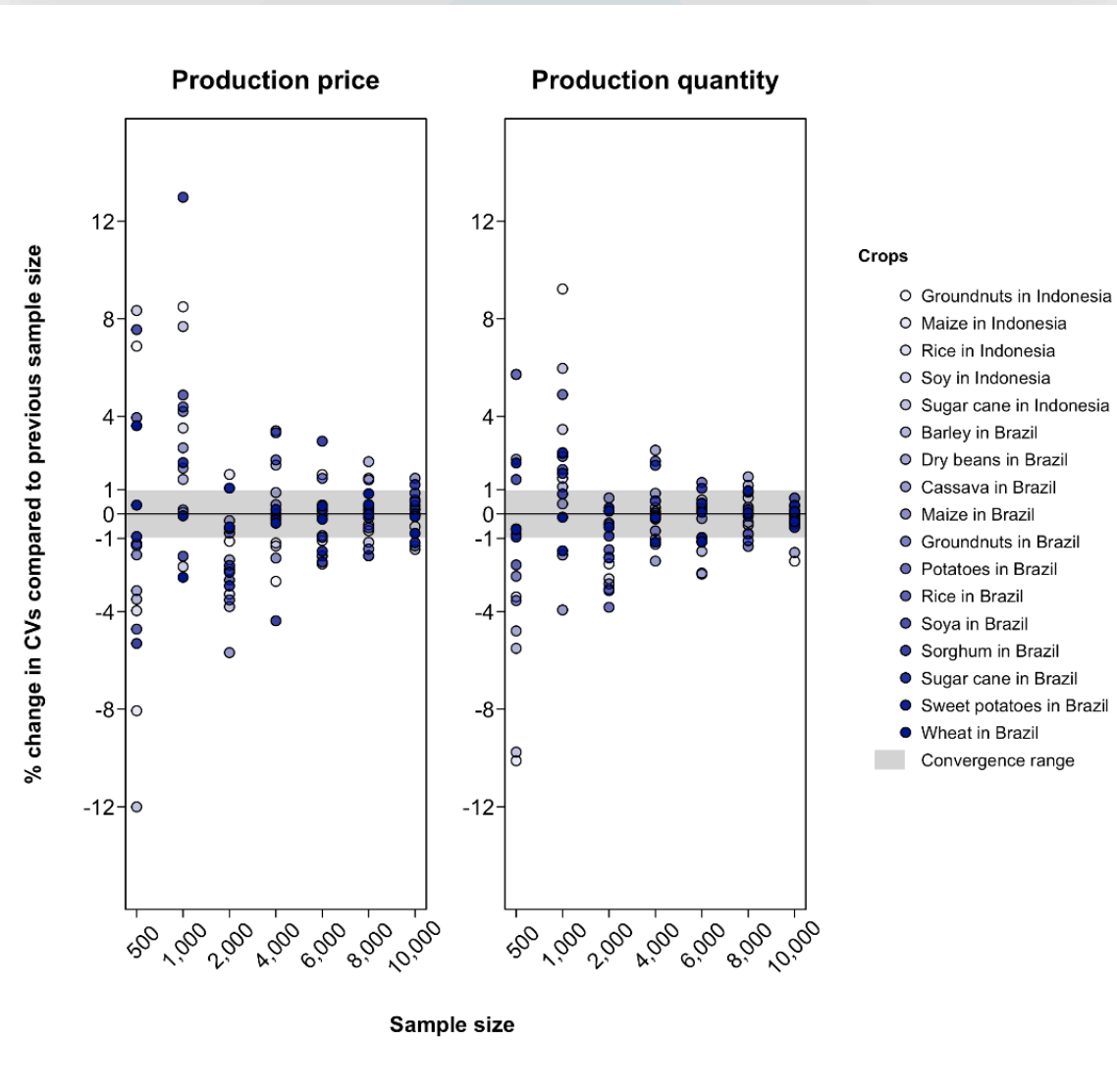
# APPENDICES



# Dynamic CGE – closure rules

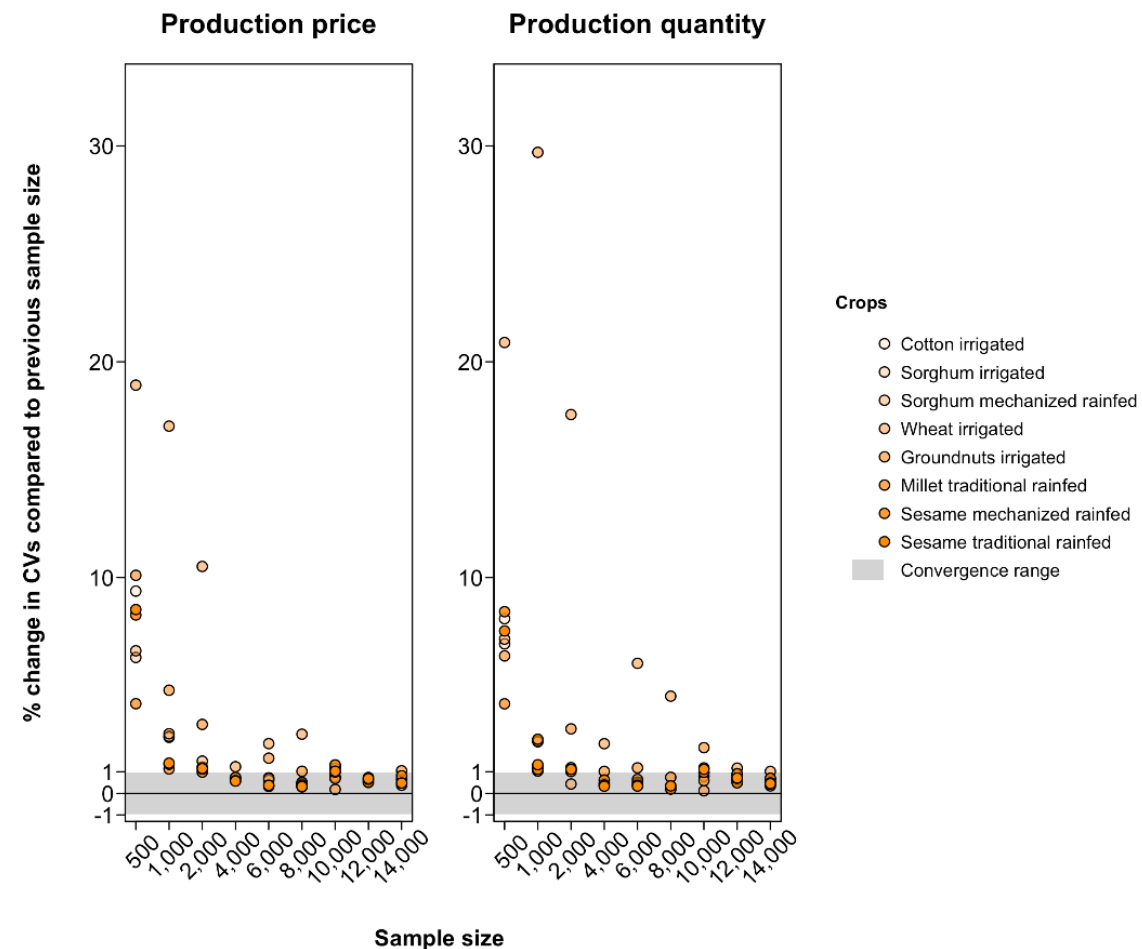
- Fixed investments as share of total absorption
- Flexible exchange rate, fixed foreign savings
- Flexible government savings and fixed tax rates
- Labour and Land - fully employed and mobile
- Capital - fully employed and activity-specific

# GLOBIOM. Benchmark



Source: Stepanyan et al. 2021

# Dynamic CGE. Benchmark



Source: Stepanyan et al. 2021

# The process of identifying good rotations

