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# Automated calibration of farm-scale mixed linear programming models using bi-level programming

Wolfgang Britz

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Editor: Thomas Heckelei		
Institute for Food and Resource Economics		
University of Bonn	Phone:	+49-228-732332
Nußallee 21	Fax:	+49-228-734693
53115 Bonn, Germany	E-mail:	thomas.heckelei@ilr.uni-bonn.de

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#### Wolfgang Britz

#### Abstract

We calibrate Linear and Mixed Integer Programs with a bi-level estimator, minimizing under First-order-conditions (FOC) conditions under a penalty function considering the calibration fit and deviations from given parameters. To deal with non-convexity, a heuristic generates restart points from current best-fit parameters and their means. Monte-Carlo analysis assesses the approach by drawing parameters for a model optimizing acreages under maximal crop shares, a land balance and annual plus intra-annual labour constraints; a variant comprises integer based investments. Resulting optimal solutions perturbed by white noise provide calibration targets. The approach recovers the true parameters and thus allows for systematic and automated calibration.

**Keywords:** Linear Programming, Mixed Linear Programming, Calibration, Bi-Level Programming, Farm-Scale Model

**JEL classification:** C61 (Optimization Techniques, Programming Models, Dynamic Analysis), Q12 (Micro Analysis of Farm Firms, Farm Households, and Farm Input Markets), C88 (Other Computer Software)

#### 1 Introduction

A stronger focus of agricultural policy on agri-environmental interactions and on the differentiated farm-scale impacts of policy instruments depending, for instance, on endowments with land, labour and capital and their quality has renewed the interest in farm-scale programming models (cf. Britz et al. 2012). Here, two strands can be observed in literature. The first builds on Positive-Mathematical Programming (PMP, Howitt 1995, for a recent review see Heckelei et al. 2012). By introducing non-linearities PMP allows for interior solutions and calibration of models where the number of binding constraints is lower than the number of non-zero variables subject to calibration. That led to PMP based programming models with a quite limited constraint set. Such models operate at the aggregate level of regions (cf. Britz and Witzke 2012) or farm types inside regions (cf. Gocht and Britz 2011) or at single farm level (cf. Louhichi et al. 2015), covering single sub-national units, nations or group of nations such as the EU (Britz and Witzke 2012, Louhichi et al. 2015). Their simulation behaviour is to

a large degree determined by the non-linear terms. This motivates a body of literature dealing with estimating and calibrating PMP type models (cf. Merel and Bucaram 2010, Howitt et al. 2012) including efforts to bridge the gap between econometric work and programming models (cf. Jansson and Heckelei 2011, Arata and Britz 2019). This is termed "Econometric Mathematical Programming" (EMP) by Buysse et al. 2007, for a review see De Frahan 2019. Here, parameters of non-linear programming models are estimated in their FOC, the cited applications estimate dual cost functions. This paper links to this body of literature by exploring the application of EMP to Linear Programming (LP) and Mixed Linear Programming (MIP) models.

LP and MIP approaches are more common for more detailed so-called bio-economic farm-csale models, for a review see Janssen and Ittersum 2007. Here, the allocative response depends solely on the interplay between the linear objective and the linear constraints: as any (not degenerate) solution is always on the corner of the constraint set, changes in a simulation imply a jump from one such corner to another. Furthermore, in any LP solution, the number of variables away from their bounds in a solution is at most as high as the number of binding constraints. LP model hence requires a rich constraint set to avoid highly specialized solutions. Integer variables e.g. related to investments, are more common than in PMP type models, leading to MIPs.

The seminal paper by Howitt 1995 on PMP provides the cornerstone on a systematic view on calibration of programming models by focusing on the FOC. Accordingly, calibration minimizes or even completely removes differences between marginal costs and revenues at the calibration point. Here, a two-step approach is common both in price endogenous market and farm-scale models. First, a data fusion step combines and corrects data from different sources to build up a data base fitting into the model's equations. For farm scale models, this step ensures at least a feasible solution with regard to constraints for which coefficients are considered fixed. While data balancing for market-scale models requires typically advanced balancing techniques (cf. Rodriguez 2014), farm scale models rely mostly on simpler approaches such as scaling resource coefficients to remove infeasibilities. Once a data set suitable for calibration is available, a second step, often called benchmarking, choses parameters are considered as fix and given, such as substitution elasticities. The others are chosen such that behavioural and productions functions replicate observed quantities at observed prices, both in market-scale and PMP models based on FOCs.

In opposite to the growing literature on the estimation or calibration of PMP based models, little has been published on calibration of constraint-rich farm-scale models, which might also reflect their declined use after the emergence of PMP. Troost and Berger 2014 report in detail on a systematic approach not applying PMP. Jayet et al. 2020 in their model documentation describe the calibration of the Europe-wide farm type LP Aropaj as "The calibration algorithm is based on sequential

calculations, combining Monte-Carlo and gradient methods. In practice, randomization of calibration parameters alternating with 'local' gradient based improvement of the criterion is generated from a large number of LP runs for each of AROPAj farm groups." While the authors report which parameters are subject to calibration (maximal cropping shares, feed requirement, livestock life cycle) and how squared differences from observed acreages, herd sizes and feed use are weighted to define the penalty to minimize, the reference above is all detail given on the algorithm itself beside reporting that between 1,000 and 2,000 runs of each LP are performed.

We develop in here a generic bi-level based programming approach which penalizes deviations from a-priori distributions both of parameters and of error terms between simulated and observed values. The paper is organized as follows. We next present an algorithmic approach discussing how to systematically remove infeasibilities, to calibrate the model and to avoid degenerate solutions resulting from calibration. The approach estimates (selected) parameters of a LP or MIP under some maximizing behaviour. We follow with applications to two smaller farm-scale didactic models, a LP and MIP. We test and assess the algorithm on variants of these models, solved for one or simultaneously for multiple years. In the latter case, degrees of freedoms do not longer allow for perfect calibration. Specifically, we randomly generate parameters for the model, add normal distributed white noise of different variance to its optimal solution and use the algorithm to calibrate the model against these observations. We assess the achieved calibration fit, the computing load and if the algorithm recovers in average the original parameters. After presenting these applications, we discuss before we summarize.

#### 2 Methodology

This section comprises three interlinked parts. We will first introduce the bi-level estimation framework; next address how to deal during calibration with constraints where both the RHS entry and resource coefficients are considered fixed, and finally introduce a modification to the objective function which reduce the step-sizes of the marginal cost curves in the LP to improve calibration.

#### 2.1 General setup of bi-level problem

As in Howitt 1995, we start with the following gross-margin maximization problem at farm scale:

$$\max_{x} \sum_{j} gm_{j} x_{j}$$
  
s.t.  $\sum_{j} a_{ij} x_{j} \le b_{i} [\alpha_{i}]$   
 $x_{j} \ge 0$  (1)

With x being the vector of non-negative decision variables indexed with j, b the constraint vector indexed with i,  $\alpha$  the related duals, gm the vector of coefficient function entries (gross margins) and a the coefficients related to the constraints<sup>1</sup>.

The PMP literature mostly discusses the case of perfect calibration against one observation of acreages and herd sizes as decision variables, typically treating the coefficients a as fix. Applications of EMP such as Arata and Britz 2019 estimating with degrees of freedom introduce error terms on decision variables. We will do the same in here such that observed levels might not be perfectly matched. A necessary condition for calibration of non-zero decision variables x in (1) is the balance of marginal revenues and marginal costs, potentially considering multiple observations t:

$$gm_{j,t} - \sum_{i} a_{ij} \alpha_{i,t} = 0 \tag{2}$$

This fundamental requirement is the cornerstone of PMP. Replacing the linear objective by, for instance, a quadratic one, the  $gm_{j,t}$  become a function of the decision variables in PMP which allows for interior solutions. Appropriate parameterization with regard to curvature generates a strictly convex problem and ensures that second order conditions (SOC) hold at the calibration point. Additionally, the constraints of (1) must be feasible at the observed point.

Our bi-level program relates instead to a linear model and considers (certain) entries in a, potentially elements of b, the gross margins gm and the x as observed with errors. We therefore introduce a penalty function g(x, gm, a, b) minimized under the FOCs and constraints of (1), resulting in the following bi-level program (Vicente and Calamai, 1994):

<sup>&</sup>lt;sup>1</sup> We do not explicitly treat in the following mathematical presentation the case of equality constraints, lower and upper bounds on the decision variables or the case of free decision variables, such as an activity which captures both buying and selling of a net-put. The proposed estimator covers all these cases. The case of a double bounded variable is included in the example as crop acreages are both non-negative and partly upper bounded based on maximum shares on the total land. We also have the land balance as an equality in the constraint set of our didactic model.

$$\min_{x,a,gm,b,\alpha} g(x, a, gm, b)$$
s.t
$$\left(gm_{j,t} - \sum_{i} a_{ij} \alpha_{i,t}\right) x_{j,t} = 0, all j, t$$

$$\left(b_{i} - \sum_{j} a_{ij} x_{j,t}\right) \alpha_{i,t} = 0, all i, t$$

$$gm_{j,t} - \sum_{i} a_{ij} \alpha_{i,i} \leq 0, all i, t$$

$$\sum_{j} a_{ij} x_{j} \leq b_{i}$$

$$x_{j} \geq 0$$

$$\alpha_{i} \geq 0$$
(3)

Bi-level problems were first introduced by Stackelberg and are mainly used to optimize some leader strategy subject that the followers' optimal answer. But they can be equally applied to an estimation framework. In (3), the inner problem comprises the constraints and FOC of model (1). The outer problem is the estimator which "proposes" parameters to the inner one. This "responds" by returning the optimal primal and dual solution x,  $\alpha$  at these parameter values or by reporting the infeasibilities. This process in encapsulated in here completely in a gradient based solver. The applications of EMP by Heckelei and Jansson 2011 or Arata and Britz 2019 are formally equal to (3) but relate to problems with a quadratic objective.

What makes our application different is that, firstly, multiple constraints are inequalities, and, secondly, that there is no second-differentiable production (or cost respectively profit) function which guarantees a unique solution to (3) and/or helps to reduce non-convexities in the solution space. Secondly, the number of inequalities is large compared to the number of decision variables, a typical feature of bio-economic models. Thirdly, we also consider the case of integer variables.

In opposite to the linear model (1), the resulting bi-level calibration problem (3) comprises cubic equality and quadratic in-equality constraints: the parameters a, the decisions variables x and the duals  $\alpha$  are estimated simultaneously and their products occur in its first three constraints. The first two cubic expressions are not strictly convex. They express FOC in the Karush-Kuhn-Tucker (KKT) form due to non-negativity conditions on x and the fact that (some) resource constraints are inequalities such that the related duals  $\alpha$  can be zero. The non-convexities render solution of such a bi-level problem numerically demanding. One aim of our paper is therefore to present an algorithm to improve the application of bi-level programming approaches to the calibration of LPs and MIPs.

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We will below present didactic applications with negative degrees of freedom where more parameters are estimated than elements of x entering the penalty function such that perfect calibration will be most likely possible<sup>2</sup>. Solving simultaneously for more multiple years leads to positive degrees of freedom where perfect calibration is not possible. The bi-level problem (3) captures hence the continuum between classical (prefect) calibration and an econometric estimation of parameters of the Leontief production function in (1) under the assumption of profit maximizing behaviour.

#### 2.2 Data balancing

The PMP literature rarely discusses cases where (1) is infeasible at the calibration point, probably as PMP based models typically have a limited constraint set. Indeed, in many, besides a land balance, only constraints relating to policy instruments such as production quotas or set-aside obligations act as a (direct) binding constraints to the production mix (cf. FFSIM: Louhichi et al. 2010; IFM-CAP: Louhichi et al. 2015). In detailed bio-economic models, infeasibilities are more likely to occur. Note here that (3) comprises the constraints of the model used for simulation (1) such that it will also (try to) remove any infeasibilities implied by the coefficients *a* and the RHS vector *b* at the observed point *x*.

If not all *a* and *b* are subject to calibration or bounds on them used, feasibility and thus perfect calibration cannot be guaranteed. We therefore minimize first squared differences between the calibration targets  $\widehat{x_{j,t}}$  and a feasible solution  $x_{j,t}$  in a separate data balancing step (4). This sub-model comprises solely the constraints comprising fixed coefficients, in here the land balance and maximal crop shares. This provides a new solution  $x_{j,t}$  where perfect calibration is at least technically feasible. In real world models, this sub-model might comprise constraints relating to compulsory policy instruments where resource coefficients and RHS entries are fixed and given by the law book.

$$\min_{x} g(x) = \sum_{j,t} (x_{j,t} - \widehat{x_{j,t}})^{2}$$
  
$$\overline{b_{i}} - \sum_{j} \overline{a_{ij}} x_{j,t} \ge 0, \text{ some } i, \text{ all } t$$
  
$$x_{j} \ge 0$$
(4)

Using only the subset of constraints where coefficients are considered fixed keeps the constraints linear and allows including integer variables in (4) as modern MIP solvers also work efficiently for

<sup>&</sup>lt;sup>2</sup> As we will discuss later, degenerate solutions are commonly found and will mean that perfect calibration in the strict sense is not possible. See next section.

linearly constrained problems with a quadratic objective. Using (4) also reveals the impact of a-priori fixing some coefficients on the calibration process. Subsequent calibration steps should be judged against the solution of (4) and not against the original targets  $\widehat{x_{j,t}}$ . (4) can be dropped if all coefficients *a* and *b* are subject to calibration and their bounds do not prevent perfect calibration or if sub-perfect calibration is accepted. The link of (4) to the bi-level problem (3) is threefold. First, the fixed coefficients in (4) will also be fixed in (3) and second, we will judge in the following to fit achieved by (3) against the solution of (4), and third, (4) provides a preliminary estimate for integer variables.

#### 2.3 Avoiding degenerate solutions

For any vector of shadow prices  $\alpha$ , there exists a vector of gross margins *gm* balancing the exhaustion conditions (2) for the non-zero elements of *x*. The number of variables away from their bounds will never exceed the number of binding constraints (not considering the bounds) in a LP. Linear dependencies generated by (3) are therefore quite likely for underdetermined problems. In that case, some decision variables can be shifted away from the calibration point(s) and others adjusted to keep the constraints feasible without changing the objective value. This is one reason why non-linearities are introduced in PMP.

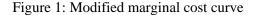
Here, we borrow the idea of PMP to introduce some costs increasing in x, using a step-wise linearization approach as proposed by Schmid and Sinabell 2005. We introduce gross margin depression effects from more specialized programs by reducing gross margins stepwise by not more in total than 1% of their expected mean; from a zero crop share to the maximal share allowed. These small gross margin changes should hardly impact the allocative response of the model and could in real-world applications be based on empirical evidence, e.g. considering preceding crop effects. Let  $gmRed_{j,t,gmd}$  [ha] measure the amount by which crop j in year t exceeds an entry in *critShare*, a matrix of given crop specific shares at which a further gross margin depressions gmd occur.  $b_{land}$  depicts the available land [ha] and gmDepr [€/ha] the changes in gross margins related to *critShare* at step gmd such that the farm's total gross margin  $gm^*$  to maximize now becomes:

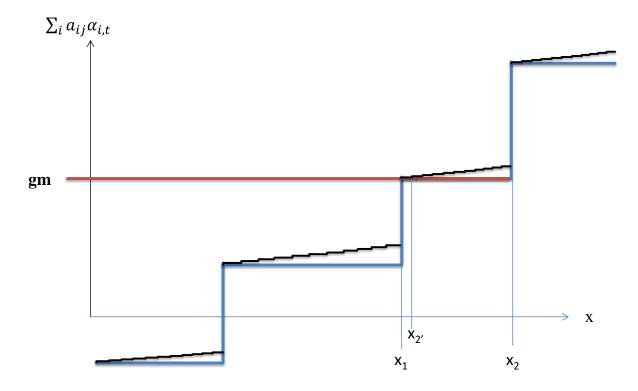
$$gmRed_{j,t,gmd} \ge x_j - critShare_{j,t,gmd}b_{land}$$

$$gm^* = \sum_{j,t} \left( x_{j,t} \overline{gm_{j,t}} - \sum_{gmd} gmRed_{j,t,gmd} \overline{gmDepr_{j,gmd}} \right)$$
(5)

The terms  $x_{j,t}gm_{j,t}$  in the new objective function shown in the second line capture the gross margins of each crop between a zero share and the first element of *critShare*, the second term stepwise decreases each crop's gross margin when its share grows. Assume 100 critical shares 1%, 2%....100% and a maximal gross margin change of 1% of 500  $\epsilon$ /ha, i.e.  $5 \epsilon$  /ha in total. This results in a uniform decrease in gross margins of 5/100 = 0.05  $\epsilon$ /ha in each depression step and provides a stepwise

linearization of a quadratic relation between the gross margin of a crop gm and its acreage x. By using non-uniform gross margin decrements, any other convex relation might be recovered. We opt for an approach which increases the step-width up to the maximal allowed crop share. The resulting larger gross-margin changes at smaller crop shares are deemed favourable in calibration as they reduce relative errors.







In Figure 1, the blue curve indicates the marginal costs before introducing the terms  $\sum_{gmd} gmRed_{j,t,gmd}gmDepr_{j,gmd}$  in the objective and the black one after their integration. The modification to the objective function reduces the step-width of the stepwise marginal cost curve of the LP. This dampens the unwanted impact of a potentially degenerate solution resulting from calibration where the primal solution can move between neighbouring points of the solution space without changing the objective. Such a case is depicted in Figure 1 where at the given gross margin gm, the decision variable can move between the points  $x_1$  and  $x_2$ . This range is reduced by the modification to  $x_1$  and  $x_2$ . This stabilizes the bi-level estimation framework as moving variables by more than the current step-width according to (5) will imply some small changes in the overall gross margin (steps on the black marginal cost curve in Figure 1). When referring in the following to (1) and the related bi-level problem (3), these problems comprise the (updated) equations from (5), i.e. the additional inequalities defining gmRed and the updated objective function and its FOC.

#### **3** Technical implementation and restart heuristics

We describe in the following three key elements of the putting the bi-level estimation to work. First, the use of a specific package in GAMS which eases its formulation and solution, second, how to detect primal degenerate solutions, and third, how to improve in case the solver only finds a local optimum in the non-convex solution space by systematically restarting the solving with different start values.

#### 3.1 Implementation and solving of the bi-level problem

Our didactic example is encoded in GAMS (General Algebraic Modelling System), a set-driven Algebraic Modelling Language easing the translation from mathematical notation into computer code. GAMS provides also transparent interfaces to solvers to efficiently solve the LP or MIP (1) and the bilevel NLP problem (3). Program control features such as loop and if-else blocks and in-built functions allow us to perform the Monte-Carlo analysis presented below. The code is found in the annex.

In order to generate problem (3) from an existing model (1), the resource constraints would need to be copied into new equations where they are additionally multiplied with their duals. Additionally, the FOC with regard to the variables would need to be coded. These tasks can be cumbersome and error-prone for detailed bio-economic farm-scale models comprising hundredth of different variables and equations. Furthermore, gradient based solvers for NLP problems will easily fail on the not strictly convex KKTs in (3). This is why specialized solvers are used for Mixed-Complementary Problems (MCP). Such MCP problems do not comprise an objective function as in (3). We therefore draw on the Extended Mathematical Programming package (EMP, Ferris et al., 2009) and the NLPEC solver (Ferris and GAMS 2009). We only need to define the simulation model (1) and the penalty function g(x, gm, a, b) in GAMS as this package allows, inter-alia, automatic formulation of the FOCs of a bilevel program. The NLPEC solver then provides different smooth approximations of the KKT conditions to overcome convexity issues. It delegates the generated bi-level program to a multipurpose NLP solver. So far, not many applications of this package to economic problems are found in literature (cf. Britz et al. 2013, Kuhn et al. 2016, Arata and Britz 2019).

Before solving the bi-level problem, we optimize model (1) at current parameter values. This provides a feasible starting solution to (3) as all FOCs of the lower model are satisfied and no constraints are violated. From there, the solver starts its search towards a better solution by updating parameters. We use the so-called penalty formulation offered by EMP package the which moves the KKT conditions into the objective function of the bi-level program such that only constraints including bounds on decision variables of (1) enter (3) as constraints. We solve the problem twice, first with a weight of 1/100 for the KKT conditions in the objective (*initMu* in the NLPEC steering file). This low weight for KKT violations allows the solver to update parameters quite easily but implies that the resulting solution only represents a primal feasible solution to the LP with considerable dual

infeasibilities, i.e. the resulting solution is sub-optimal. In a second final solve, the weight for KKT violations is increased to 1.E+6 (*finalMu* in the NLPEC steering file) to remove dual infeasibilities. CONOPT4 finds a local minimum to the bi-level problem typically in a few seconds as long as the number of observations is small, benefitting from parallelism.

#### 3.2 Detecting degenerate solutions and improving on local optima

Problem (3) comprises the FOC and not the SOC which are anyhow all zero if the inner problem is a LP. This allows for (and will in many cases result in) degenerate solutions rooting in linear dependencies. Starting the gradient based solver used for (3) also on the simulation model (1) after fixing the parameters to its own estimates should let the solver accept its own solution as the optimal one. This hides potential degeneracy. Therefore, after solving (3), we reset all decision variables to zero and solve the LP at the estimated parameters with the specialized solver CPLEXD to check for deviations. In case of integers being present, they will be unfixed in this solve which can provoke additionally differences between the optimum of the bi-level problem and the subsequent solve of (1).

Finding a global optimum for a bi-level programming approach where the inner problem comprises inequalities and bounds is computationally challenging. Improved calibration of the model typically requires switching the slack status of multiple inequality constraints. Non-binding constraints have no impact on the duals or the feasibility status. A gradient based solver will typically not consider changes in the RHS or coefficients in currently non-binding constraints if larger updates are required to do render them binding. It will therefore tend to find a local optimum only, depending on its start values. To improve here, we need an additional algorithm which offers different start points to the gradient based solver even if no integers are present. This implies an additional outer loop generating starting points for the gradient based solver.<sup>3</sup>

With a sufficiently small parameter space, systematic search algorithms such as a grid search might be used for this outer loop. As already smaller changes in parameters can have a larger impact

<sup>&</sup>lt;sup>3</sup> We repeatedly switch between five variants of the perturbation. The first two perturb based on the current best set of parameters, only, multiplying each parameter with N(1,0.05) and N(1,0.10), respectively. The third one multiplies it with N(1,0.10) and adds N(1,0.01) times the a-priori mean of all parameters. Similarly, the fourth one multiplies the current best parameters with N(1,0.50) and adds N(1,0.10) times the a-priori mean to others. The last one only uses the expected mode of the parameters, adding u(-0.5,2.5). These choices are clearly arbitrary and the outcome of some testing. Still, as they are defined relative to the expected parameter modes and current best parameter values, they can be used with other problems as well.

on the model's fit, this would require a quite fine-grained grid. Already three grid points such as [lower bound, mode, upper bound] for each of the twenty parameters in our model would mean 3^20 tries which is computationally impossible. We draw here instead on the algorithm proposed by Schäfer and Britz 2019 which construct restart points by perturbing stochastically the current best parameters (see also Figure 3).

The outer-loop requires at least a maximum number of re-starts of the bi-level problem as a stopping criterion, here chosen as hundred. This is a relatively small number which allows test many model instances in combination with multiple calibration targets in the Monte-Carlo analysis described in the next section. In applications to an actual model, a higher number might be appropriate. Beside restriction the maximum number of starting points, one might stop testing further restart points once a parameter set offers a satisfactory fit, here defined solely based on the deviations from the calibration targets and no considering deviations from expected parameters values:

$$fit = \frac{1}{T * J} \sum_{j,t} (x_{j,t} - \widehat{x_{j,t}})^2$$
(6)

The fit is not measured based on the solution of (3) returned by the solver. Instead, we reset all x reset to zero and, potentially, unfix integers and solve the primal model (1) at the parameter estimates. Restarts might therefore even occur under a perfect fit reported by the bi-level estimator in case where this subsequent solve returns a different primal solution.

Repeated restarts until a very accurate threshold in (6) is reached will improve in average over many calibration exercises the fit at the cost of higher run time and vice versa. We opt here for a compromise which increases the threshold of what is considered a sufficient fit the more restart points where already tested. In the didactic application below, the fit relates to average squared deviations in ha, with acreages adding up to 100. We start with a minimal fit of zero in the first trial which is linearly increased to two when the maximal of 100 trials is used. Starting with a very low threshold will trigger restarts of the bi-level estimator even if the accuracy of early trials is already quite high to allow for cheap further improvements. We consider the chosen maximal threshold of two as sufficiently close to the "true" observations after one hundred trials; the typical fit achieved is far better as discussed below as long as the number of observations is small. Increasing the threshold slightly after each restart also reflects that perfect calibration with multiple observations is often impossible. Furthermore, as discussed in section 2.3 above, the step sizes of the gross margin changes in (5) determines ultimately the possible calibration quality.

Incorporating integer variables directly in the bi-level estimation framework is not possible with the solver available to us such that we cannot propose a generic approach for MIP problems. As long as coefficients relating to integer variables in the objective function and in constraints are treated as fixed and given, the integers can be fixed in the bi-level estimator and become free variables again in a subsequent solve of the simulation model at the currently drawn parameters to assess the fit. In our tests, the algorithm could in average considerably improve the calibration compared to the "true" parameters with integer variables<sup>4</sup> present as long as the number of observations was small. That is somewhat surprising as, once integers are present, not only the FOC must hold at the current parameter choice, but the resulting objective must also be higher than any other integer solution. This condition cannot be tested in an estimation framework for larger number of integers.

#### 4 An example application

The example application does not refer to the calibration of an existing bio-economic model against observations such as FADN. The true data generation process leading to, for instance, to the FADN observations, is unknown such that we cannot assess if the approach introduces biased parameter estimates. We therefore construct rather simple model LP and MIP models for which we draw parameters in a Monte-Carlo analysis, perturb their optimal solution with white noise and then let the bi-level estimator find parameters which calibrate them.

#### 4.1 Model setup

Our didactic model (see Table 1) comprises elements related to crop production found in many biophysical models such as land balance, maximal cropping shares, annual and monthly labour constraints and, in the version comprising integers, machinery requirements and related investments. It covers five crops. While land and yearly labour endowments as well as maximal crop shares are fixed, we generate variants based on Monte-Carlo analysis where additional constraints and model coefficients differ.

Specifically, we consider different labour endowment available in three peak months as additional constraints. Each peak month has a labour endowment of 50% above the 1.000 hours annually divided by twelve months, perturbed for the variants by a uniform distribution of u(0.9,1.1). Revenues in  $\in$  per ha for each crop and year are drawn stochastically from a uniform distribution u(1000,1200) and costs in  $\in$  per ha for each crop from u(400,500). We infer from there labour needs per hour by making an assumption how much of the total gross margin of the farm remunerates land. The remainder of the total gross margin is used to estimate a shadow price per labour hour and to derive an estimate of total labour needs per ha from revenue exhaustion for each crop. The total annual labour needs for each crop serve as a basis to allocate labour need shares to the three peak months, multiplied with

<sup>&</sup>lt;sup>4</sup> The GAMS code comprises the necessary code to test the discussed extension of the model with integer variables and the changes in calibration set-up.

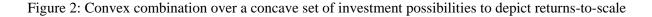
u(0.75,1.25). In each year, we have hence ten potential constraints (land, four labour constraints, five maximal cropping shares) and five decision variables.

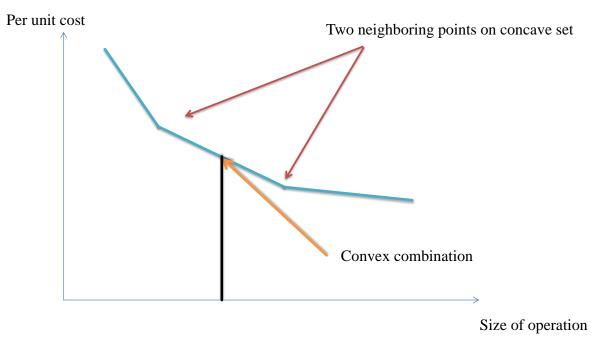
Model block	Elements	Details		
Decision variables and objective function, LP	Five crop acreages for 1 to 10 years	Revenues differ by year (fixed), variable cost time independent (MC)		
Decision variables and objective function, MIP	As above, integer based investments into different machine by type and size, once for all years	Machinery costs and yearly operation capacity (fixed)		
Constraints	Land balance	RHS: 100 ha (fixed)		
	Total annual labour	RHS: 1000 hours (fixed); crop specific labour needs (MC)		
	Labour in three peak months	RHS: 1000 hours / 12 times * 1.5 (+MC); crop specific labour needs (MC)		
	Maximal crop shares	Fixed		
	Machinery needs (only MIP)	Fixed		

Table 1: Characteristics of didactic models subject to Monte-Carlo analysis

Note: Element indicated as fixed are not subject to calibration, MC: element is subject to Monte-Carlo analysis to test calibration of different variants of the same structural model

In the model version with integer variables, we introduce machinery requirements covered by investments taken for the whole period. We consider five different machine types of different sizes [10,50,100], where the size refers to the acreage in ha which can be operated in each year. Related annual investment costs are [1000,4000,6000]  $\in$  which implies costs of [100,80,60]  $\in$  / ha and year at full capacity use, i.e. increasing returns-to-scale. For each machinery type, a convex combination between neighbouring points of the concave set is endogenously chosen, where the chosen points are depicted by integer variables (see Figure 2). Machinery requirements at farm level are defined as the total acreage covered by the crops needing the machine, in average over the years. Further details can be found in the GAMS code in the annex and in the supplementary material.





#### Source: Authors

Equation (7) below depicts the penalty function g(x, gm, a, b) as chosen in this test application. As the decision variables are acreages, their entries into the land constraint are unity and these coefficients are not subject to calibration. The same holds for the maximal crop shares. Labour demands and the per hectare costs *c* are subject to calibration, they don't carry an observation index, while we treat the RHS vector *b* as given.

We introduce as the first term in the penalty function absolute squared differences between the simulated  $x_j$  and observed acreages  $\hat{x_j}$ , identical to (6). Second, we add relative squared differences between the estimated per ha cost  $c_j$  and the "true" parameters  $c_j$  in the penalty function, and finally, squared relative differences for the resource coefficients subject to calibration:

$$\min_{x,c,a,\alpha} g(x,c,a) = w_x \sum_{j,t} \left( x_{j,t} - \widehat{x_{j,t}} \right)^2 + w_c \sum_j \left( \frac{c_j - \widehat{c}_j}{\widehat{c}_j} \right)^2 + w_A \sum_{i,j} \left( \frac{a_{ij} - \widehat{a}_{ij}}{\widehat{a}_{ij}} \right)^2 \tag{7}$$

The weights  $w_x$  for the calibration of the *x* are as in (6);  $w_c$  referring to the per ha costs *c* is equal to the number of crops, and the weights for the resource coefficients subject to calibration  $w_A$  is equal to the number of constraints. Note that in a real world application, one would probably also use relative deviations for the decision variables if these are of different magnitudes.

In order to test the calibration process, we first solve the model at the true parameters. Next we add white noise error terms with differing  $\sigma^2 = [2,5,10]$  to the resulting optimal solution of the "true" model  $x_{true}$  to generate random calibration targets:

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$$\widehat{x_{l,t}} = x_{l,t}^{true} + n(0,\sigma^2) \tag{8}$$

The follow-up data balancing step ensures that calibration targets do not violate the maximal crop shares, the land balance and non-negative conditions which related to coefficients which are not subject to calibration. This step minimizes the first term of (7), targeting the outcome of (8):

$$\min_{x} g(x) = \sum_{j,t} (x_{j,t} - \widehat{x_{j,t}})^{2}$$
s.t.
$$\sum_{j} x_{j,t} = b_{land}$$

$$0 \le x_{j,t} \le maxShare_{j}$$
(9)

The data generation process resulting from (8) and (9) cannot generate  $x_{j,t}^{true}$  in average where some crops will be frequently zero. Adding errors terms in (8) and truncating at zero in (9) will bring such zero observations in average over the draws into the solution. The land balance will then imply downward bias for non-zero observations. When the model is solved simultaneously for multiple years, revenues *r* per hectare change stochastically across years, while none of the coefficients subject to calibration carries an observation index. If perfect calibration is possible at all will depend on the number of time points used as discussed in the next section.

There is a trade-off in (7) between the calibration fit and staying close to the mode of the parameters. One might set the weights in front of the parameters to zero to arrive at uniformed priors for the parameters. That is however dangerous as e.g. the overall farm gross margin is not controlled during estimation. If the *c* entries for all crops are changed by the same absolute amount, the dual of the land constraint as an equality will change accordingly. There are hence likely linear dependencies in the model. That problem can be partly avoided by removing the land balance and its dual value from the lower level and move the land balance in the upper level in (3). After the solution, the costs of all crops can be reduced by an assumed land rent. A similar approach was used by cf. Kanellopoulos et al. 2010 in a PMP model. We consider here the more usual case where a priori information on the parameters is used and duals are not explicitly controlled.

#### 4.2 Set-up of the tests and assessing the performance of the estimator

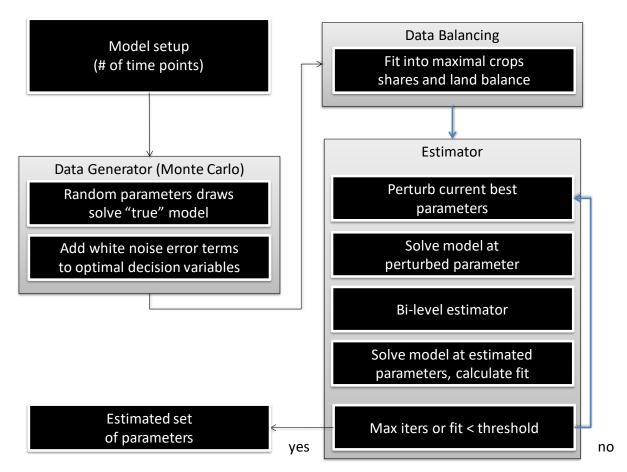
We set-up the model such that it comprises one or multiple years (see also Figure 3). For each number of years, we generate fifty model variants by randomly drawing parameters, i.e. yearly revenues, and time invariant costs and four labour requirements for each crop. Maximum crop shares and farm endowments besides labour availability in peak months remain unchanged. For each variant we first determine the optimal solution. From there, we generate twenty different calibration targets by adding white noise error terms to the optimal solution for all crops, including unobserved ones. We hence

consider the LP as the true data generation process. We explore to what extend the algorithm recovers in average the true parameters while at the same time test its calibration performance. For each number of years and the different variances of the error terms tested in the model, this implies 1.000 draws (fifty different sets of parameters times twenty different error terms). For each draw, we allow the search algorithm up to hundred perturbations of the parameters and related restarts of the solver on the bi-level problem to find a best-fit set. As discussed above, the required fit to stop the search process increases linearly from zero for the first try to two.

For each instance and draw, we solve the data balancing problem (4) and use its solution as the calibration target in (7). We next (a) perturb the current best solution of the parameters, (b) solve the primal model (1) at fixed resulting parameter values, (c) unfix the parameter and solve (3) (at fixed integers in case of the MIP model), (d) fix parameters to its solution, set decision variables to zero, unfix the integers in case of MIP and solve problem (1) from where we measure the fit. If the fit is above the threshold or the maximal number of restarts not yet reached, we repeat (a)-(d).

The twenty randomly drawn labour requirements and five cost entries in the objective are parameters subject to calibration. Jointly with the number of observations and crops, they determine the degrees of freedom. A model comprising one year, only, and five observed crops acreages suggests an undetermined model with twenty free parameters. However, bounds on the parameter, in-equalities and non-linearities in (3) do not allow defining exactly the degrees of freedom. Already with two years, (almost) perfect calibration was not always possible. We face ten FOC conditions with two years and lose for each of the potentially four binding labour constraints in each year one degree of freedom as one of the crop specific coefficients is depending on the others. Jointly with bounds on parameters, that explains why there might be cases where perfect calibration is impossible even with two years. For such cases, the algorithm acts as Bayesian estimator where the structure of the model and the observations jointly determine the posteriori of the parameters and the error terms. Minimizing squared relative differences of the parameters in combination with some weights to express a-priori information is a rather intuitive approach. Formally, under normal distributed errors, the approach maximizes the log-likelihood of the posterior density (Heckelei et al. 2008) which further motivates its use as the penalty function. The quadratic function with its linear derivatives is also a good choice for gradient based solvers. Other penalty functions such as (cross)-entropy approach could be used as well.

#### Figure 3: Overview on methodology



#### Source: Authors

We assess the algorithm firstly by its ability to calibrate the model sufficiently accurate based on the average fit. The efficiency of calibration is evaluated based on the number of restarts which strongly impact computing time.

#### 4.3 Results

We test the case of one year (= one observation) for different standard deviations of the white noise error added to the "true" model solution to assess the performance of the algorithm. With one observation, the coefficient of variance for the estimated parameters is in the one to five percent range, depending on the variance of the error term, and mean deviations from the true ones below one percent (see Table 2). Some deviations can be expected due to bias in the data generation process discussed above which also implies some bias for the estimated parameters.

	N(0,2)	N(0,5)	N(0,10)
Dente contr	-0.1282	-0.0967	-0.0769
Per ha costs	(0.015,-0.0001)	(0.016,-0.0001)	(0.014,-0.0001)
	+0.0004	-0.0086	-0.0071
Labour per ha, total	(0.010,+0.0002)	(0.012,-0.0007)	(0.012, +0.0009)
Labour per ha, July	-0.0019	-0.0071	-0.0081
	(0.027,-0,0002)	(0.031,-0.0042)	(0.033, -0.0048)
	0.0057	+0.0044	+0.0071
Labour per ha, August	(0.025,+0.0056)	(0.028,+0.0045)	(0.031, +0.0066)
Labora ang ba Santonghan	0.0008	+0.0019	+0.0019
Labour per ha, September	(0.020,+0.0016)	(0.030,+0.0030)	(0.030, +0.0030)

Table 2: Mean error, coefficient of variance of error and mean relative error of estimated parameters, no integers

Note: Parameter statistics are expressed as average over crops; coefficient of variance (first) and mean relative mean error (second) in brackets. Column headings refer to the white error noise added to the optimal solution of the variant.

Against that background, the almost perfect fit might be astonishing, even more so the low coefficients of variance. The size of the error term seems also to have a very limited impact on the statistics. This might firstly reflect quite limited stability ranges of the drawn solutions, i.e. relative small changes in coefficients of the "true" simulation model lead to larger changes in the primal solution. Secondly, the maximal crop shares determine to some extent the solution. For a crop bouncing against the upper limit in the "true" case, a positive perturbation will mean that data balancing based on (5) will pull them to or close to the upper limit. We might hence expect similar effects in models with a richer constraint set narrowing down the solution space.

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	N(0,2)	N(0,5)	N(0,10)
	0.022	0.026	0.027
Fit of simulation model	(0-0.19)	(0-0.33)	(0-0.26)
Fit of hi lovel estimator	0.0027	0.0013	0.0004
Fit of bi-level estimator	(0-0.19)	(0-0.15)	(0-0.24)
Error term	2.02	12.95	48.80
	(0-12.07)	(0-94.00)	(0-299)
Fit improvement	-94.65%	-97.73%	-98.65%
# of starts	2.04	2.27	2.57
	(1-13)	(1-16)	(1-18)

Table 5. Quality of fit and required restarts for the case of one observation, no integers	Table 3: Quality of fit and required restarts for the ca	ase of one observation,	no integers
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Note: (1) Fit measured as squared deviations between calibration target and solution in ha, divided by number of observation, i.e. five, reflecting the number of crops. (2) First number in each cell is the mean; min and max in brackets. (3) The error term measures the average squared deviation of the calibration target from the uncalibrated model solution. (4) Fit improvement: relation between fit of calibrated model and uncalibrated one as expressed by the error term.

The average fit of the calibration with one observation (see Table 3) above does almost not respond to the average size of white noise errors error added and is very small with just 0.022 to 0.027. The calibration fit which can be achieved reflects, as discussed above, the step-width of the gross margin depression mechanism. The average fit of the bi-level estimator suggests that it is almost always possible to find a parameter sets for which the FOC hold at the calibration target. Increasing the variance of the error term has a very moderate impact of the performance of the estimator. There are no considerable differences in the fit from a model application perspective, i.e. the fit of the simulation model, or with regard to required restarts of the model, when the average distance between the "true" model and the calibration target increases considerably.

As expected, introducing integer variables renders calibration harder (see Table 4): it drives up the required average restarts substantially and reduces considerably the fit. This also reflects that the threshold increases dynamically with the number of restarts, i.e. if the algorithm does not find a good fit after a few restarts, it will also consider a lower fit as sufficient to stop further searches.

Overall, the results suggest that an acceptable calibration might also be possible in case of integer variables. Introducing integers *reduces* in here the average error term but worsens the fit and drives but the number of required restarts. The reason is the returns-to-scale effect which favours more specialized solutions where crops hit more often their maximal cropping shares or don't enter the optimal solution. The data balancing step might be pushed in some instances towards the simulated

solution. The reduced fit is not so astonishing as the parameters related to the machinery requirements restrictions which are linked to the integers are not under control of the estimator.

	N(0,2)	N(0,5)	N(0,10)
Fit of simulation model	0.227	0.650	1.615
Fit of simulation model	(0-6.64)	(0-32.97)	(0-61.95)
Eit of hi lovel estimator	5.526	4.757	1.254
Fit of bi-level estimator	(0-1105)	(0-1559)	(0-179)
Error term	1.958	12.622	46.857
	(0-12.11)	(0–98.23)	(0-349)
Fit improvement	-81.20%	-93.56%	-95.03%
# of starts	14.51	18.46	23.22
	(1-100)	(1-100)	(1-100)

Table 4: Quality of fit and required restarts for the case of one observation, integers included

Note: for explanations, see Table 3.

We test the case of multiple observations (i.e. a simultaneous solution for multiple years) only for the case of N(0,2), for results see Table 5 which also comprises for comparison the case of a single observation. The average number of restarts with two observations increases from around 2.42 to around 2.97 while the fit worsens only slightly to 0.048. This might still be considered a perfect calibration in terms of average squared differences in ha for a farm with 100 ha. A drop in the calibration performance with multiple observations is expected. In the case of one observation, only, the per ha crop costs alone can be used to solve for the FOC of type (2). Calibration in case of two or more observations requires updates to other coefficients as well. Parameter updates will change the primal solution if they relate to binding constraints, only, and will typically impact the fit of all years simultaneously. In case of two observations, there was one draw out of the thousand with a larger error term where the algorithm could not find any solution improving the fit. In case of three observations, larger calibration errors are quite common reflecting the fact that degrees of freedom seem regularly exhausted.

With higher number of time points, the problem is no longer undetermined for many of the draws. That reduces the average fit. Due to the dynamic thresholds in the outer loop of the algorithm, this also implies in average more starts of the solver. Still, for up to five observations, the fit of the calibrated model is substantially improved compared to the uncalibrated one.

# of obs.	Fit of simulation model	Fit of bi-level estimator	Error term	Fit improvement	# of starts
	0.022	0.0027	2.02	04.55%	2.04
1	(0-0.192)	(0-0.19)	(0-12.07)	-94.65%	(1-13)
	0.048	0.020	2.17	-96.90%	2.97
2	(0-6.06)	(0-6.06)	(0.01-8.62)		(1-100)
2	0.114	0.076	2.17	04.070/	6.03
3	(0-3.33)	(0-2.78)	(0.06-7.75)	-94.07%	(1-100)
5	0.259	0.210	2.08	86.250/	11.73
5	(0-1.60)	(0-1.58)	(0.19-6.07)	-86.35%	(1-67)
10	0.792	0.760	2.05	-60.98%	30.76
10	(0.15-1.96)	(0.12-1.93)	(0.55-3.94)		(1-75)

Table 5: Quality of fit and required restarts for different number of observations, no integers

Note: for explanations, see Table 3.

The impact of introducing integer variables on the fit and more so on the required restart is much stronger as seen from Table 6. The integers with their related constraints restrict the solution space considerably further compared to the model above and drive the model towards more specialized solutions. This implies that the changes to the parameters subject to estimation are less likely to allow fitting to given calibration targets which differ from the model solution at the "true" parameters. The solution at the true parameters clearly also reflects the integers and related constraints. Furthermore, integers are fixed to their optimal values at the currently drawn parameter values during estimation such that the estimator cannot consider that other integer values might become optimal if parameters are updated. This becomes only visible in the subsequent solve of (1).

Already with five observations, finding solutions with a good fit with integer present takes very long and we were not able to run the fifty variants times twenty randomly derived calibration targets<sup>5</sup>.

<sup>&</sup>lt;sup>5</sup> Each trial required from a few to several ten seconds to solve. With 50x20 Monte-Carlos and each Monte-Carlo draw subject to up to 100 restarts with perturbed parameter sets, the time requirements became prohibitive for larger number of observations. One reason was that CONOPT4 went sometimes into infinite loops which required breaking that solve manually such that the processes could not run completely unintended. Generating all results required more than a week despite solving different tests in parallel.

In many cases, even hundred restarts could not deliver a fit better than the maximal considered threshold of two.

# of obs.	Fit of simulation model	Fit of bi-level estimator	Error term	Fit improvement	# of starts
	0.227	5.526	1.958	01.100%	14.51
1	(0-6.64)	(0-1105)	(0-12.11)	-81.199%	(1-100)
2	0.470	3.267	2.092	74.950/	26.72
2	(0-8.01)	(0-846)	(0.01-10.76)	-74.85%	(1-100)
2	0.579	6.442	2.098	70.50%	29.38
3	(0-6.66)	(0-1980)	(0.01-7.78)	-70.50%	(1-100)
<i>c</i> *	0.916	1.250	2.079	56 2204	38.50
5*	(0.002-4.83)	(0-187)	(0.18-5.69)	-56.32%	(1-100)
10**	1.057	1.001	1.953	47 790/	40.75
10**	(0.20-3.40)	(0.13-3.62)	(0.67-3.53)	-47.78%	(10-100)

Table 6: Quality of fit and required restarts for different number of observations, with integers

Note: for explanations, see Table 3. \* based on 33x20 experiments. \*\* based on 5x20 experiments.

Our model is quite small such that one might expect a bi-level problem with a few variables and equations, only. Due to the gross margin depression mechanism, the simulation model comprises however for each time point and crop 50 non-negative variables and inequalities. In the bi-level program, that implies 200 endogenous variables: the primal variables and related duals as well as the slacks in the equations and their duals. For five crops and five periods, that already implies 200 \* 5 \* 5 = 5,000 variables. Due to complementarity conditions, the EMP package will automatically remove some of them from the model. Still, the resulting bi-level estimation problem for five time points comprises slightly more than 2,500 equations and 5,000 variables.

#### 5 Discussion

Compared to PMP, the proposed calibration method has a different focus. In PMP, the coefficient matrix is usually taken as fix and given while non-linearities are introduced to capture "unobserved" costs or revenues. We consider instead objective function entries and (some) resource coefficients as observed with errors and minimize these errors during calibration. If the model subject to calibration likely misses constraints faced by the farmer and/or in other cases of (other) unobserved costs or revenues, a PMP approach might be more appropriate. Another difference to PMP is that we refrain

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from structural model changes which strongly impact its allocative response. The proposed gross margin depression mechanism is deliberately parameterized such that it "just" allows for "interior" solutions while largely maintaining the step-wise marginal cost curves of the original LP. PMP instead deliberately overwrites the solution behaviour of a LP with a low number of constraints. Closed-form solutions (c.f Merel and Bucaram 2010) are now available to calibrate different types of PMP models against (certain sets of) price elasticities. In our framework, price elasticities could be used to introduce observations with updated prices and decision variables. The usefulness of calibrating the allocative response of a *single* farm model again elasticities is open to debate as most available elasticity estimates capture average responses in a farm population and are likely to vary across farms.

Using our approach with a higher number of observations is a special case of EMP where profitmaximal parameters of a Leontief production function are estimated. Compared to e.g. Arata and Britz 2019 the estimator faces in our examples more inequality constraints and is tested also for the case of integers. Resulting non-convexities in the solution space of the bi-level problem require res-start heuristics to find better local optima. This cannot guarantee a global optimum but is found to improve considerably the fit. Besides a maximal number of restarts, we used a minimal fit as a stopping criterion in our large-scale Monte-Carlo analysis. This might not be necessary in real-world applications to fewer cases where also more restarts could be used. Alternatively, one might experiment with so-called global solvers, an option we discarded after tests did not look promising. We conclude from our tests that the heuristics work quite well with pure linear models but that no general conclusion can be drawn in presence of integers. The model layout with investments decisions for multiple machines in different sizes required by different sets of crops depicted as integers proved quite challenging for larger number of observations but preformed still quite well with one or two.

Troost and Berger (2014) discuss an alternative approach using real-world observations to calibrate a larger set of MIP programming models. While they consider somewhat more parameter as uncertain compared to our didactic application example, they consider also 0-1 parameter choices such as "if all agents face either unlimited or zero demand or supply of these goods". In total, they tested around 2.400 parameter combinations from which they fixed only those which in all three observation years could improve some aggregate measure of fit across the around 500 farms. For the rest, they conducted large-scale uncertainty analysis simulation experiments. Thus, their approach aims mostly at excluding some parameters from this step. Its advantage is firstly that the individual models need no to be technically integrated into one problem as in our approach. Indeed, each single of their models has many thousands variables and equations which might exclude a simultaneous bi-level estimation framework. Secondly, it can be used with MIP models where coefficients related to integers are considered uncertain. But their approach clearly cannot calibrate individual models (almost) perfectly.

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A detailed comparison to the approach of Jayet et al. 2020 is not possible with the available information. They also consider selected resource coefficients as uncertain – but as it seems not objective function entries - and improve model calibration of each instance independently by testing in some systematic way different parameter sets.

The true data generation process is unknown in real-world application. Data on production processes on farm (crop nutrient requirements, necessary field operations and related machinery and labour needs, feed and stable place requirements etc.), knowledge on likely constraining endowments (land, labour, machinery, buildings, water rights etc.) and assumptions on optimizing behaviour are the elements in building a detailed bio-economic model. This information typically stems from a mix of sources, such as data from official statistics, often at the level of administrative units such as for prices or crop yields, farm accounting data, farm planning handbooks, field experiments, questionnaires, econometric work etc., (cf. the discussion of parameterization in Troost and Berger, 2014). Many of the resulting model parameters are not directly observed for the farm instances subject to calibration. Furthermore, observed yields, netput quantities, prices etc. might deviate from expectations used when allocative decisions were taken. That renders it inviting to consider larger ranges of many parameters as uncertain but runs the risk of overfitting model instances during calibration. Still, besides a well-motivated model structure and parameterization, a satisfactory fit against multiple observations provides more or less the only indication to what extent a bio-economic model provides a good representation of the real technology and decision behaviour.

Working with algorithms which provide a systematic approach to calibration such as the one proposed in here increase transparency in calibration. They require clear decisions on what parameters are changed up to what range and on relative weights used to penalize deviations from given calibration targets and the starting parametrization. Our findings suggest that, firstly, the proposed algorithm is able to recover the true parameters in Monte-Carlo experiments and, secondly, that it enables quite accurate calibration as long as degrees of freedom allow for it. As such, there is some confidence that a parameterization resulting from its application is a reasonable choice against the background of the chosen settings such as calibration targets and assumed distributions of parameters and errors terms. A further advantage is that it can be entirely encoded in GAMS, a software widely used in field of farm-scale programming models. Indeed, we were able to apply the approach also successfully in the highly detailed bio-economic farm model FARMDYN (Britz et al. 2016).

#### 6 Summary and conclusion

We present a rather universally applicable algorithm which calibrates a (farm-scale) LP or MIP model drawing on the idea of PMP (Howitt 1995) by systematically adjusting uncertain coefficients in the model, but without introducing new structural elements such as non-linear "unobserved" costs. The

aim here is to base the allocation steering solely on the interplay of the linear objective and the (rich) constraint set of the model. As such, the approach is hardly suitable to most models where now PMP is applied. We apply a bi-level estimation approach where the outer problem controls the fit of the calibration and the lower problem is the actual simulation model, represented by its FOCs. Technically, we use the EMP package of GAMS in combination with the NLPEC solver to automatically convert the simulation model into its FOC. However, due to the non-convex solution space and the presence of integer variables, the application of a gradient based solver to find local minima is combined with heuristics to generate starting points from existing good solutions.

We exemplify the application with a simple didactic model with a land balance, several labour and maximal crop share constraints; a variant of this model introduces machinery requirements linked to integers depicting investments in machines. The approach is tested in a systematic way by starting with known model parameterizations and related optimal solutions, for different number of observations. We perturb the optimal solutions by white noise, next apply some data balancing step as one would also expect in a real-world application (e.g. to render observations consistent to maximal crop shares and given land) and next calibrate the model against the resulting observations. For just one observation, we find (almost) perfect calibration in all tests. With growing number of observations, we move away from an underdetermined model such that the algorithm searches a bestfit parameter set, but still, in average, allows for a quite accurate calibration against the perturbed observations. Jointly with the GAMS code of the example found as an annex, the presented approach opens the door for more transparent, systematic and automated calibration of farm-scale programming models. It was also successfully tested with the quite detailed bio-economic farm model FARMDYN (Britz et al. 2016) to calibrate it to crop shares and animal herds.

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