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The concepts and quantification of yield gap using boundary lines. A review

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ABSTRACT

Context: The potential yield of crops is not usually realised on farms creating yield gaps. Methods are needed to diagnose yield gaps and to select interventions. One method is the boundary line model in which the upper bound of a plot of yield against a potentially limiting factor is viewed as the most efficient response to that factor and anything below it has a yield gap caused by inefficiency of other factors. If many factors are studied, the cause of the yield gap can be identified (yield gap analysis, YGA). Though the boundary line is agronomically interpretable, its estimation and statistical inference are not straightforward and there is no standard method to fit it to data.
Objective: We review the different methods used to fit the boundary line, their strengths and weaknesses, interpretation, factors influencing the choice of method and its impact on YGA.
Methods: We searched for articles that used boundary lines for YGA, using the Boolean "Boundary*" AND "Yield gap*" in the Web of Science.
Results: Methods used to fit boundary lines include heuristic methods (visual, Binning, BOLIDES and quantile regression) and statistical methods (Makowski quantile regression, censored bivariate model and stochastic frontier analysis). In contrast to heuristic methods, which in practice require ad hoc decisions such as the quantile value in the quantile regression method, statistical methods are typically objective, repeatable and offer a consistent basis to quantify parameter uncertainty. Nonetheless, most studies utilise heuristic methods (87% of the articles reviewed) which are easier to use. The boundary line is usually interpreted in terms of the Law of the Minimum or the Law of Optimum to explain yield gaps. Although these models are useful, their interpretation holds only if the modelled upper limit represents a boundary and not just a particular realization of the upper tail of the distribution of yield. Therefore, exploratory and inferential analysis tools that inform boundary characteristics in data are required if the boundary line is to be useful for YGA.
Conclusions and implications: Statistical methods to fit boundary line models consistently and repeatably, with quantified uncertainty and evidence that there is a boundary limiting the observed yields, are required if boundary line methods are to be used for YGA. Practical and conceptual obstacles to the use of statistical methods are required. Bayesian methods should also be explored to extend further the capacity to interpret uncertainty of boundary line models.

1. Introduction

The development of high-yielding crop varieties is critical to the global food security because global population is expected to rise while the area of land available for agriculture is shrinking (Mueller and Binder, 2015). This increased potential yield, however, is not always realised in actual production. This is known as the yield gap. The yield gap has taken centre stage in discussions about global food security (Giller et al., 2021; Timsina et al., 2018; van Ittersum et al., 2016), and if crop improvement objectives are to be met, agronomists must understand this gap and identify interventions to close it. Therefore, methods for understanding crop yield variability and unraveling the underlying factors that cause the yield gap are urgently needed.

The yield gap is defined in reference to some benchmark yield and here we consider three such benchmarks, the potential yield, the water-limited potential yield and the attainable yield. The potential yield is defined as the genetically-possible yield of a cultivar grown in non-limiting biophysical and environmental conditions i.e. under an

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optimum supply of water and nutrients, in the absence of biotic stress and with optimal agronomic management i.e. sowing dates, sowing density, weeding and so on (van Ittersum and Rabbinge, 1997). However, under field conditions in rainfed cropping, crop growth may be limited by water supply, hence the potential yield is reduced to the water-limited yield potential. While management interventions like irrigation can, in principle, alleviate this limitation, this might not always be feasible for the farmer. The largest yield that can be achieved under these limiting conditions in well-managed fields (i.e. with correct and timely fertiliser application rates, timely weeding, and so on) is called the attainable yield (FAO and DWFI, 2015; Tittonell and Giller, 2013). Attainable yield is sometimes estimated as 80% of the potential yield or the water-limited potential yield for rain fed systems.

Attainable yields are often not realised by farmers due to suboptimal management of biotic and abiotic factors within their control. These include yield-limiting factors like nitrogen supply, which constrain the crop's net primary production, and yield-reducing factors, such as weeds which compete for available resources and, pests and diseases, which sequester some or all of the net primary production before this is harvested. Hence, there is a yield gap between the potential yield, water-limited yield potential, attainable yield and the farmer's actual yields (Fig. 1), which could, in principle, be closed by applying appropriate management strategies (Cossani et al., 2010; van Ittersum and Rabbinge, 1997; van Ittersum et al., 2013).

To close this yield gap, there is a need to identify and rectify the potentially manageable yield-limiting and yield-reducing factors. The process of quantifying and identification of the underlying cause of yield gaps, is called yield gap analysis (Fermont et al., 2009; van Ittersum et al., 2013). The yield gap can be identified and quantified by comparing the actual yield to a reference benchmark yield, which can be the potential or water-limited potential yield predicted by a process model e.g. using the Global Yield Gap Atlas (GYGA) (see https://www.yieldgap.org). The use of process models to determine the benchmark yield depends on the assumption that the model is not significantly biased and that all factors determining yield are properly understood and quantified for a particular setting (Shao et al., 2023). An alternative is the use of an empirical approach that observes actual yields and plots them against corresponding measurements of potentially limiting factors. An example data set consisting of hypothetical wheat yield and a soil property x_i is presented to illustrate this. In a setting where farmers practice a wide range of management practices, it is expected that there will be a wide range of actual yields depending on how individual farmers manage the yield-limiting or yield-reducing factors, x_i (Fig. 2). If one can assume that the sample is large enough to include cases in which the crop is managed as well as possible, then this can be taken as the attainable yield and can be used as a benchmark yield in that particular setting (e.g 12.5 t ha^{-1} in Fig. 2).

While the attainable yield might be identified empirically, further insight into the yield gap is required to guide interventions. The interpretation of a plot of some biological response against one of several potentially limiting factors was first proposed by Webb (1972) as the boundary line model. Unlike controlled experiments, where sources of variations other than that of the factor of interest are controlled as far as possible and modelled as additive random effects allowing the fitting of a best-fit median regression model through the data scatter, non-experimental data (e.g. real farm data) have many uncontrolled sources of variation. This results in a scatter of the response variable, y, against a factor, x_i, for which there is a range of responses for a single level of the factor. As proposed by Webb (1972), this kind of plot for biological response may be interpreted in terms of an upper limit for the response which appears to depend on x_i (see Box 1). This upper limit can be modelled as a function of x_i, specifying the largest response for some value of x_i as shown in Fig. 2. The observed responses are assumed to be limited by factors other than x_i in some way and the upper limit of the response as a function of x_i represents the most efficient response (i.e. when all other factor are not limiting) for a given level of x_i, which Webb (1972) called a boundary line, $f_i(x_i)$. This gives a better representation of the relationship of y as a function of x_i than the median best fit line in this case. Points below the boundary line have a response gap equal to the difference between the actual responses and the maximum response at that level of factor x_i (Fig. 2) (Webb, 1972). A boundary line model can, therefore, be used to model the largest yield as a function of

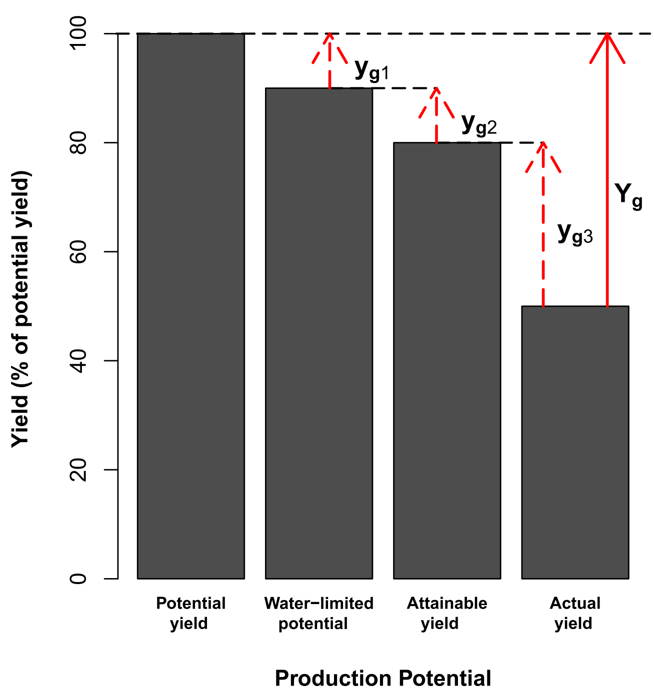


Fig. 1. Yield gap estimation using different production potentials as benchmarks. The yield difference between potential yield and water-limited potential yield (y_{g1}), water-limited potential yield and attainable yield (y_{g2}), and attainable yield and actual yield (y_{g3}) add up to the total yield gap (Yg).

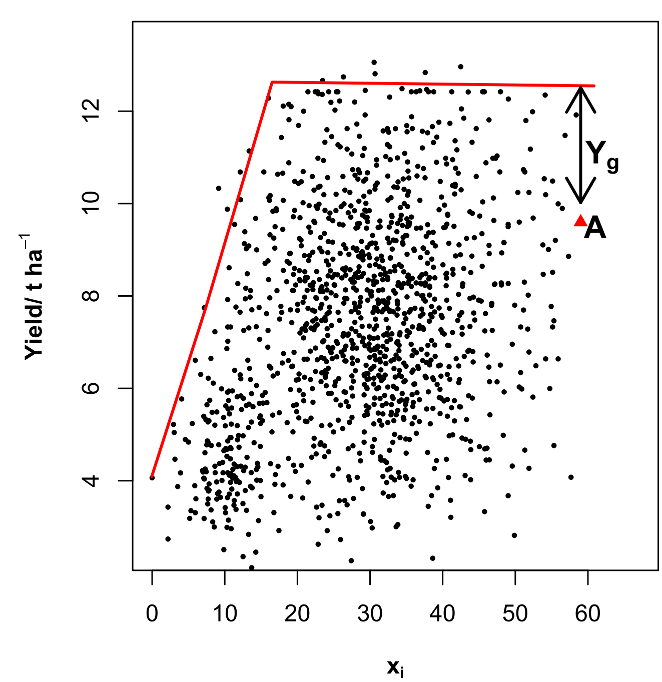


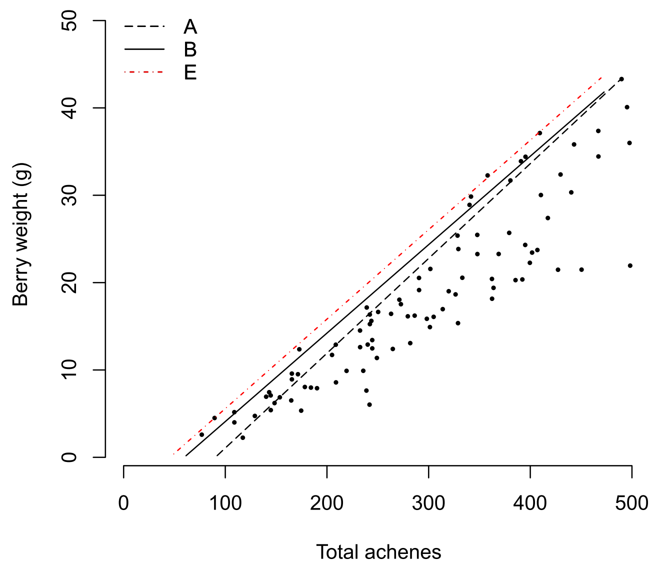
Fig. 2. A hypothetical scatter plot of maize yield against yield-limiting or yield-reducing factor, x_i, with a model (the red solid line) that predicts the maximum yield response that can be achieved at a given level of factor, x_i. Yield gap, Y_g, is the difference between the attainable yield (12.5 ha^{-1}) and the actual yield,A.

yield-limiting or yield-reducing factors and therefore, the yield gap. The largest predicted yield in a given setting represents its attainable yield (Dehkordi et al., 2020).

to what extent the different approaches provide an objective way of fitting the boundary line, their weaknesses and strengths, trends in the usage and factors influencing the choice of boundary line fitting approach, and the impact of using the different approaches on yield gap analysis.

Box 1: Existence of a boundary in biological response data (Webb, 1972)

A scatterplot for achene number against berry (pseudocarp) weight of 94 well-shaped red gauntlet strawberries from a study by Abbott et al. (1970) showed presence of a boundary beyond which response did not exceed (line E). Line A represents the boundary when only the best-developed berries were considered (six achenes per cm^2 of the surface) while line B is boundary when strawberries were grouped at intervals of 20 achenes with the heaviest berry and its associated number of achenes representing each group. This study illustrates how such an upper limit in a dataset can be treated as a standard against which average performance can be assessed, so as to arrive at an estimate of possible increase in yield Box-Fig. 1.



Box-Fig 1. Boundary line relationship between the total number of achenes and berry weight re-plotted from Webb (1972).

Additional useful agronomic information can be extracted from the boundary line model for yield gap analysis such as the contribution of different factors to the identified yield gap as has been done by many agronomic studies (e.g. Casanova et al. 1999; Cao et al. 2019; Fermont et al. 2009; Hajjarpoor et al. 2018; Kintché et al. 2017; van Vugt and Franke 2018). However, the information obtained depends on how the boundary line is interpreted, which must reflect the natural process of crop growth due to the effect of various factors. Various laws which govern how factors affect plant growth in nature have been proposed which can be used to interpret the boundary line model.

Though boundary line analysis is empirically and theoretically plausible as a basis for yield gap analysis, in practice, the estimation of the boundary line, statistical inference as to whether it can be meaningfully interpreted as an upper limit, and an account of uncertainty in parameters of the line are not straightforward (Webb, 1972). There is, therefore, a need for quantitative methods for both estimation and inference if useful information is to be obtained from the boundary line model. FAO and DWFI (2015) gives an overview of methods (that include the boundary line methodology) used to benchmark yield, giving examples, but do not give full detail on the procedures to fit the boundary line function to a dataset. Various methods are available in the literature for fitting a boundary line to a dataset. However, consolidated information on their implementation, strengths, limitations and agronomic interpretations is lacking. In this review, we give an overview of (i) the different agronomic interpretations of the boundary line that have been used in yield gap analysis and (ii) the different approaches to fitting boundary line that are available for yield gap analysis. We analyse

2. Methods for review

Peer-reviewed publications were searched using the Boolean term “Yield gap*” AND “Boundary*” applied to All fields in the Web of Science database on 1st June 2023. A total of 70 studies were obtained with this search. These studies were further screened and only publications that applied the boundary line methodology to access yield gaps were selected. Publications that applied other methods for accessing yield gaps as well as review papers were excluded ($n = 17$) resulting in 53 publications being retained. Using Google Scholar, we also searched for publications cited by the retained articles which used boundary lines for yield gap analysis but did not appear in the initial search. Eleven publications were added from this. This produced a total of 64 publications in which boundary line methods were used for yield gap analysis. The list of selected publications are listed in Table S.2 of the supplementary material. Key information extracted from these articles was stored in a database, specifically the year of publishing, crop studied, domain of study, the agronomic interpretation of the boundary line, criteria used to identify outliers, the method used to estimate the boundary line i.e whether this was based on a statistical model or heuristic method (’non-statistical’) and the assumptions made for the boundary line method used (e.g. the percentile value assumed to be the boundary for binning methods). By a heuristic method we mean one that is intuitively reasonable, but generally entails arbitrary decisions and, because it does not invoke an explicit statistical model, does not provide a natural basis for inference or the characterization of uncertainty. On the other hand, a statistical approach follows strict statistical principles and makes sound assumptions in fitting the boundary line.

3. Boundary line interpretations

In this section, we discuss how the boundary line methodology is interpreted for yield gap analysis. We focus on the principle, strength and limitations of these interpretations.

Plant growth is governed by a series of natural processes (Poorter et al., 2013). The empirical observations of the boundary line must, therefore, be interpreted in light of a conceptual model of these processes if useful information is to be obtained from them. One such conceptual model is the law of the minimum which states that a biological response can only be as large as the factor in least supply can permit (Liebig, 1840; Sprengel, 1826). This can be modelled by expressing the response, y, as a function of factors $x_1, x_2 \ldots, x_n$ as follows

$$y = k\min\{f_1(x_1), f_2(x_2), \ldots, f_n(x_n)\} \tag{1}$$

where $f_i(x_i)$ represents the boundary line response to variable x_i and for this interpretation is scaled so that its maximum value is 1, and k is a constant which represents the attainable yield in this case. If the law of the minimum holds, and the potentially limiting factors $x_1, x_2 \ldots, x_n$ take a wide range of values in the dataset, then the upper boundary on a plot of y against x_i should estimate the attainable yield scaled by the boundary line function, $kf_i(x_i)$, the largest biological response that can be attained by a given level of factor x_i given that no other factors are limiting (Lark et al., 2020). Boundary line functions, $f_i(x_i)$, for the responses of crop yield to several growth-defining, limiting, and reducing factors, $i = 1, 2, \ldots, n$, can be determined and the factor that predicts the minimum yield is viewed as the most limiting factor and therefore, the predictor of yield in that instance (Fermont et al., 2009). The identification of the most limiting factors allows agronomists to prioritize which factors need more attention to increase the yield in a given location (Wairegi et al., 2010).

Though the law of the minimum provides a simple and straightforward conceptual framework for boundary line analysis and has been used by most authors to interpret the boundary line (Cossani and Sadras, 2018; Fermont et al., 2009; Nehbandani et al., 2020; Shatar and McBratney, 2004; Wairegi et al., 2010), it does not account for possible interactions of factors associated with crop growth. That is to say, it assumes that all factors independently determine a possible yield, of which the smallest is actually attained, while in reality two or more independent variables can have a simultaneous effect on the dependent variable such that their joint effect significantly differs (greater or less) from the sum or minimum of the individual effects. One conceptual model that entails such interactions is the law of the optimum which states that the response of a dependent variable to an independent factor that is in minimum supply is largest when the other production factors are close to the optimum (Liebscher, 1895). This means that the growth response of a plant to a given factor of interest depends on a subset of other factors that interact with the factor of interest and that the response is largest when this subset is close to some optimum requirement. As an example, an intermediate process of uptake affects the relationship between the rate of nutrient application and yield. The nutrient uptake itself is also affected by other factors and hence there will be a relative change in position of the yield function in response to a rate of nutrient application due to changing conditions of factors that affect uptake. This intermediate effect of nutrient uptake considered in the law of optimum is not considered in the law of the minimum (de Wit, 1992).

The boundary line can be interpreted in light of the law of the optimum if it is thought of as a rate-limiting function, as proposed by Elliott and de Jong (1993) for the interpretation of boundary responses to soil properties of nitrous oxide emission from soil cores. The response variable, y, is influenced by the limiting factor, x_i, on the abscissa of the boundary plot, a set of other potentially limiting factors which interact with x_i, and a set of other factors which are not limiting. Therefore, the response, y, is given as a product of the function of the factor of interest and functions of factors that interact with the variable x_i.

$$y = k\prod_{i=1}^{n} f_i(x_i) \tag{2}$$

As with Equation (1), the boundary function, $f_i(x_i)$, is scaled to 1. When all factors other than the i^{th} factor on our boundary plot which potentially limits the response, y, are optimal, i.e. for any $j \neq i$, $f_j(x_j) = 1$, the response, y, will be determined by $f_i(x_i)$, and will be on the boundary of the plot of y against the i^{th} factor. If the data for the potentially limiting factors is large enough and covers a wide range of values, the function, $f_i(x_i)$, will fit the boundary of the plot of y against the i^{th} factor as illustrated in Fig. 3. The solid line represents the boundary line when all factors are optimum as the law of the optimum. If some factor(s) other than the i^{th} factor are not optimal, the boundary line will drop below the solid line as represented by a dashed line in Fig. 3. In this sense, the form of the response to the i^{th} factor is determined by the other factor(s), which is what we mean by an interaction. However, this type of interaction is a simplistic formulation as it is a product of the boundary functions and is, therefore, restrictive. In practice, more complex interaction models could be used to underpin boundary line modelling. In the form presented in Equation (2), the law of the optimum implies that observations on the boundary, below the attainable yield are subject to limitation by x_i while points below the boundary are limited by other factors. The boundary line, therefore, still allows us to identify a yield gap.

The law of the optimum which accounts for the simultaneous effect of different factors of crop growth, is more biologically plausible than the law of the minimum (de Wit, 1992). However, the rate-limiting interpretation of the boundary line has not been widely considered particularly in respect of plant growth. Out of the 64 reviewed articles, none interpreted the boundary line using the rate-limiting interpretation. This may be because the law of the optimum, on which the rate-limiting interpretation is based, has not been widely investigated since it was suggested by Liebscher (1895). A possible approach to account for interaction is the use of boundary surface models from

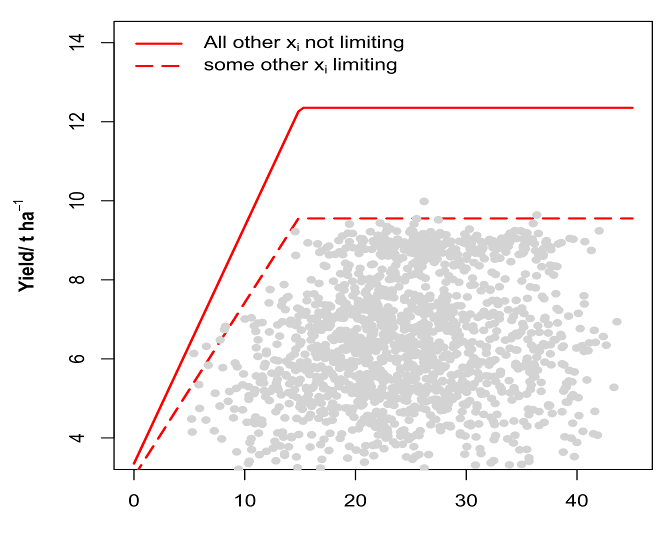


Fig. 3. The illustration of the law of the optimum for boundary line interpretation. The solid line represents the most efficient response of yield to factor x_i when all other factors are optimum and hence represents the boundary line response to x_i, while the dashed line represents the function of the response of yield to factor x_i when some other factors are not optimum.

multi-dimension plots similar to the response surface methodology (Myers et al., 2016). A boundary surface model would represent the maximum attainable yield for combinations of values of potential limiting factors, and a range of functional forms would be possible, including both additive and interactive effects. This approach has been used in plant nutrition studies to optimize nutrient application rates (Jahan and Amiri, 2018; Salawu et al., 2007). However, we are currently not aware of any study that has attempted to use response surfaces by fitting multi-dimension boundary lines to account for interaction.

Interaction has been incorporated in boundary line analysis in other ways including the use of nutrient ratios (nutrient balance indices) rather actual individual nutrients to plot the data. The importance of balanced nutrition (e.g. N:P, N:S, C:N, K:Mg) has been emphasised in agronomic literature (Duncan et al., 2018) as the deficiency of one nutrient might restrict the efficient use of another (Aulakh and Malhi, 2005). Use of these ratios reflects the combined effect of two factors on yield and hence interaction. However, ratio models are based on prior knowledge, and are not a general method to represent interaction of factors. The co-limitation framework (Cossani et al., 2010; Cossani and Sadras, 2018) has also been used to account for interaction in boundary line analysis (Carciochi et al., 2020). Co-limitation occurs when two factors simultaneously limiting plant growth (Riar et al., 2016). This interactive effect has been determined through the use of resource stress indices. A resource stress index (e.g. nitrogen stress index) is a measure of the level of stress experienced by the crop due to limitations in essential resources and is determined by subtracting from one, the ratio of the resource uptake at actual yield to the uptake at potential yield (Cossani et al., 2010). Individual stress indices are used to calculate various degrees of co-limitation which have then been used to evaluate their effect on observed yield gaps from boundary lines (Carciochi et al., 2020).

The boundary line interpretation using the law of the minimum and the law of the optimum provides useful agronomic information that helps to identify the causes of the yield gap and how they can be addressed. Silva et al. (2017b) introduce in addition to the potential yield (Y_p), the attainable yield (Y_a) and the actual yield (Y_r), the technically efficient yield (Y_t), which is the maximum yield attainable given x_i and here equal to the original unscaled $f_i(x_i)$-the boundary value. Note that Y_t is defined only when $f_i(x_i) < Y_a$, i.e. when $f_i(x_i) < f_i(\widetilde{x}_i)$ where $f_i(\widetilde{x}_i) = Y_a$.

The efficiency yield gap, g_e is

$$g_e = f_i(x_i) - Y_r, \qquad f_i(x_i) > Y_r \tag{3}$$

$$g_e = 0, \quad f_i(x_i) = Y_r \tag{4}$$

This gap indicates that some factor(s) other than x_i limit crop yield and so action is required to remove this limitation. If these limitations are removed, then the expected yield is $Y_t = f_i(x_i)$. The efficiency gap, g_e implies that any resource used to sustain factor x_i at its observed level e.g fertilizer or labour, is inefficiently used as the actual yield could be sustained at some $\breve{x}_i$ where:

$$f_i(\breve{x}_i) = Y_r < f_i(x_i) \tag{5}$$

if g_e were zero, but $f_i(x_i) < Y_a$ then there is a resource gap.

$$g_r = Y_a - Y_t \tag{6}$$

The resource yield gap is attributed to the fact that $x_i < \widetilde{x}_i$, so if, for example, x_i is an available nutrient, then some resource (e.g. fertilizer)

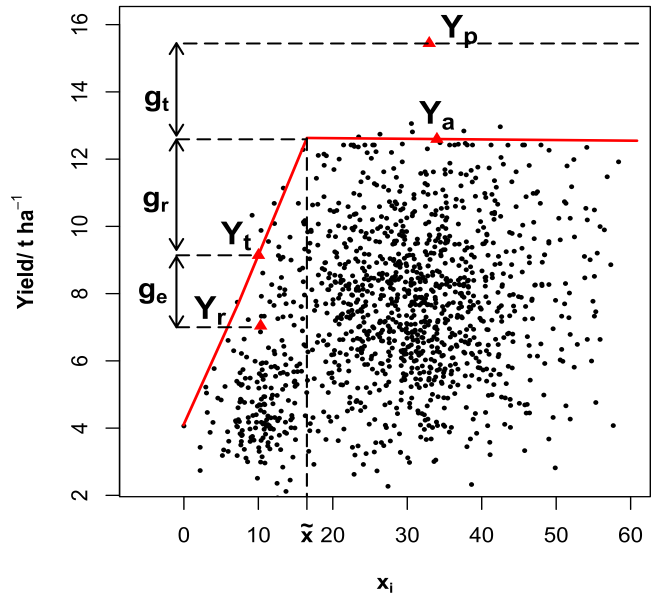


Fig. 4. Decomposition of yield gaps into efficiency (g_e), resource (g_r) and technological (g_t) yield gaps. Y_p is the potential yield, Y_r is the actual yield and Y_t is the technically efficient yield given the limitation of x_i. The level of factor at which the yield reaches attainable yield is given by $\widetilde{x}_i$.

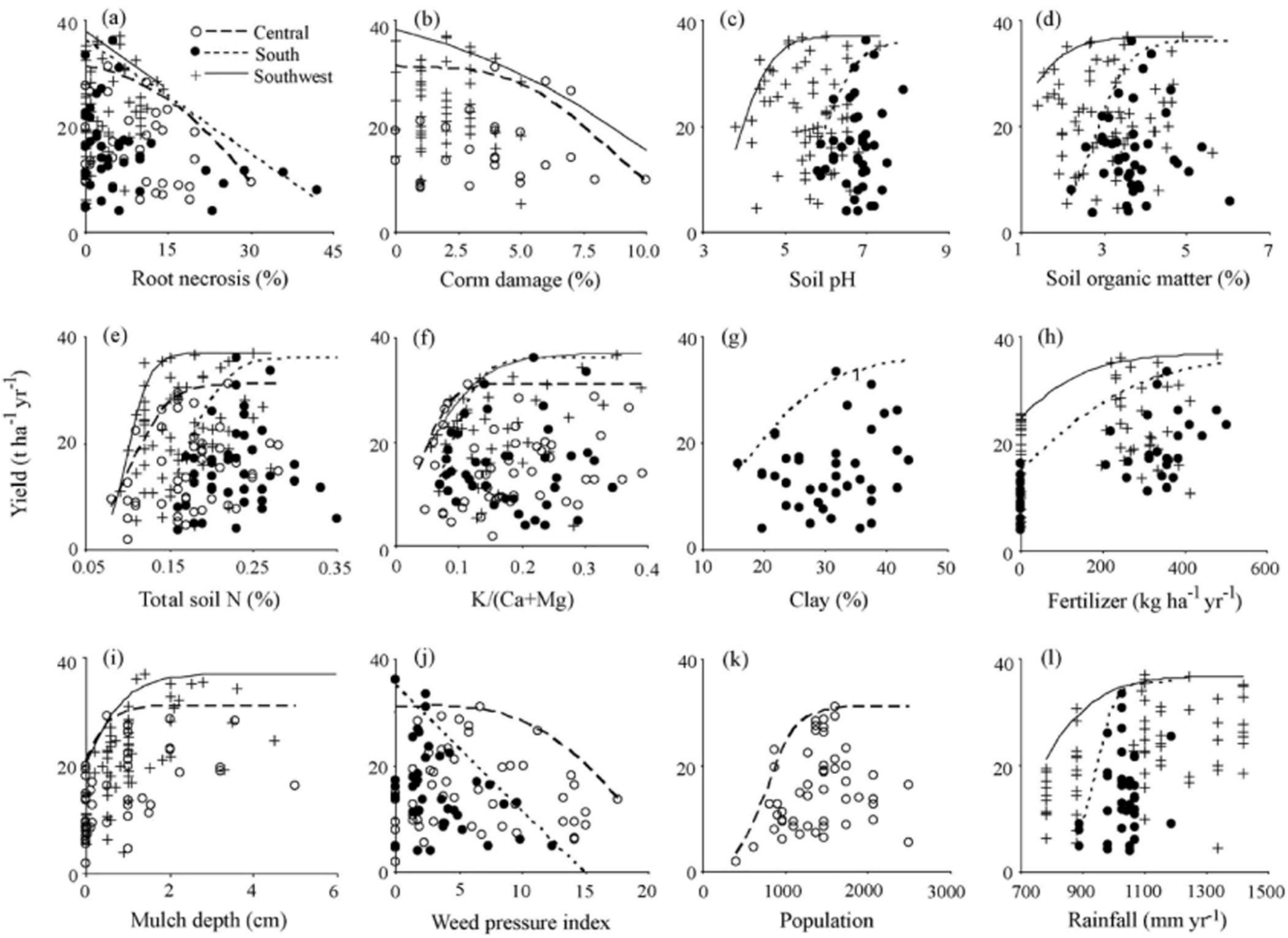
must be used to close the gap. This is because it is assumed that all other factors are optimum and hence there is a maximum response to factor x_i. If the law of the minimum is considered, however, some other factors may become limiting as you increase the factor x_i and hence the yield may fall below the technically efficient yields (Fig. 4).

The technology yield gap (g_t) is the difference between the potential yield (Y_p) and the attainable yield (Y_a). This gives a measure of how much room there is to increase the yield if improved technologies are applied like the addition of an irrigation system or the growing of crops in a controlled environment like a greenhouse.

When the boundary line is applied to several factors that affect yield in a given location, one is able to check if one of the factors considered can explain the identified yield gap (Box 2). The explained yield gap, as illustrated in Fig. 5, can be quantified as the difference between the attainable yield, Y_a, and the largest yield predicted by the most limiting factor while unexplained yield gap can be quantified as the difference between the largest yield as predicted by the most limiting factor and the actual yield (Fermont et al., 2009; Wairegi et al., 2010) as shown in Fig. 5(b). Given a set of actual yields measured simultaneously with two soil factors A and B as shown in Fig. 5, we can select one particular farm with actual yield, Y_r, and show it on the plot of the two soil factors. It can be seen that the total yield gap is approximately 9.5 t ha^{-1}. Factor B is the most limiting factor as it predicts a smaller yield, Y_{lim} (approximately 8.5 t ha^{-1}), as compared to factor A (12 t ha^{-1}). The unexplained yield gap will, therefore, be the difference between Y_{lim} and Y_r as there are unknown factors that need to be addressed for Y_r to be increased to Y_{lim}. Once these unknown factor are addressed, increasing the yield from Y_{lim} to Y_a can be achieved by increasing the level of factor B and therefore, this is referred to as explained yield gap.

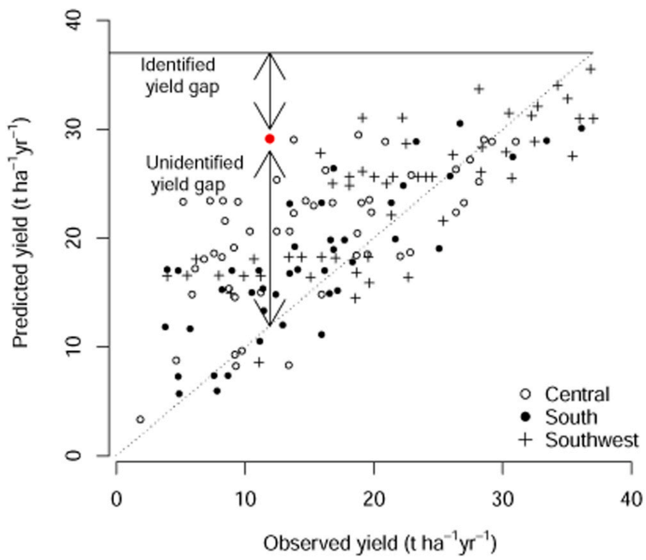
Box 2: Explaining yield gaps in East African highland banana systems (Wairegi et al., 2010)

A study was carried out to identify the factors limiting banana production in Uganda. Banana yield data for different farms were collected in central, south and south-west regions of Uganda and a variety of limiting factors including soil pH, SOM, Total-N, K, Ca, Mg, nematodes, weevils, weeds, plant population and rainfall were also measured. Boundary lines were estimated for each factor (Box-Fig. 2).



Box-Fig 2. Boundary relationship between banana yield and biophysical factors in Uganda (Wairegi et al., 2010).

The expected yield for each farm was then estimated using the boundary lines and the factor that predicted the lowest yield was taken as the most limiting factor. Yield gap estimation and decomposition was conducted by plotting the predicted yield using boundary lines against the actual yields as shown in Box-Fig. 3. The continuous line at 37 t ha^{-1} yr^{-1} represents the highest yield observed in the study area and it is taken as the attainable yield. The 1:1 dotted line represents the situation when the actual yield is equal to the predicted yield. The points that fall above the 1:1 line means the predicted yield by the most limiting factor is larger than the actual yield and therefore, its yield gap cannot be explained by any of the factors investigated in the study. The yield difference between the predicted and attainable yield can be explained by the most limiting factor. For example, taking the yield represented by the red dot above the 1:1 line, the unidentified yield gap of 18 t ha^{-1} yr^{-1} while the explained yield gap is 7 t ha^{-1} yr^{-1}. In this way, they were able to identify which factors were mostly limiting yield in the area and which one could be prioritised to increase banana yields.



Box-Fig 3. Observed and predicted yield from boundary line approach replotted from Wairegi et al. (2010).

4. Estimation of boundary line function and its statistical inference

In this section, we discuss the process of fitting a boundary line function, $f_i(x_i)$, as described in Section 3 to an $\{x, y\}$ scatter plot. We first discuss the importance of statistical inference about the boundary line model for yield gap analysis and then we explore the different methods currently available for fitting the boundary line function to data.

4.1. The need for statistical inference about boundary line functions for yield gap analysis

We have shown that the boundary line model can be interpreted consistently with two different conceptual models. Under either model, the boundary function may be useful for developing practices and interventions to close the yield gap as illustrated by our cited examples. However, we must also consider whether the boundary line interpretation is supported fully by the data (FAO and DWFI, 2015). After all, a boundary could be drawn by hand on any plot of some y and x variable, including the familiar model where deviations of y from some $f(x)$ are independent additive random effects. Even if one of the conceptual models holds, some of the variation in y is likely to behave as additive random variation, specifically the measurement error for the crop yield, or other response.

Milne et al. (2006b) developed an exploratory approach to this hypothesis in which the density of points in the upper section of successive convex hulls (peels) of data in $\{y, x_i\}$ space is compared with the same statistic for a null model with additive random effects only. The convex hull of the data in a 2-D scatter plot is the smallest subset of the data which constitute a convex subset containing all the observations (Skiena, 2008). All the points in a convex hull of a data set comprise the first "convex hull peel". The second peel is the convex hull of the remaining data after the first peel is removed. If a boundary exists for which responses cannot exceed, it is expected that the data will have a distribution that has a denser concentration of points than normal near the boundary (upper convex hulls). The distribution will take the form of a censored bivariate distribution. Otherwise, if a boundary does not exist, the data is likely to follow a bivariate normal distribution with randomly distributed points some of which lie at the extreme fringes. The data points at the extreme fringes arise due to random additive error associated with the effect of other factors affecting response other than the variable of interest as in a general linear model with additive random effects. This can be taken as a null model against which a boundary line model can be tested. This method is, however, less powerful as it is based on just the number of vertices in the peels ignoring the distribution of the peels at the upper bounds of the data.

This work by Milne et al. (2006b) is the first of which we are aware that attempted quantitatively to test the plausibility of a boundary model. We suggest that further work is needed on exploratory and inferential analysis to test the plausibility of boundary models if they are to be used to interpret data in terms of yield gaps and provide recommendations. It should also be noted that the interpretations from boundary line analysis are conditional on the support of the data (i.e. if the yields and environmental variables are field means, farm means, or means for small plots within fields) (FAO and DWFI, 2015). Results at different scales may differ as additional constraints may apply more at one scale compared to another.

4.2. Methods for fitting boundary line functions

The reliability of the information obtained from a boundary line model is dependent on method used to fit the boundary line function. A good fitting method must possess three important qualities. Firstly, it should be objective (Schnug et al., 1995; Shatar and McBratney, 2004) as this ensures that the results are consistent, reproducible and can easily be compared. Secondly, the method should be able to account for measurement error in response variables and allow quantification of uncertainty of the boundary line (Lark et al., 2020; Makowski et al., 2007; Milne et al., 2006a). Finally, as noted in the previous section, the method should allow some objective test against a null (non-boundary) alternative to check if a boundary exists within a dataset (Lark and Milne, 2016; Lark et al., 2020; Milne et al., 2006a).

Despite the increasing use of the boundary line approaches in the agronomic literature (see Fig. 8(a)), there is no standard protocol to estimate a boundary line for yield gap analysis (Hajjarpoor et al., 2018; Shatar and McBratney, 2004). Many methods currently in use to derive the boundary line follow a similar process of (i) Plotting a scatter for dependent against independent variables, (ii) removal of outliers (iii) selection of the boundary data points, and (iv) fitting a boundary line to the selected points which may take the form of a linear model, broken-stick model or non-linear model. Important difference amongst the methods are the criteria used to identify outliers, the procedure used to select the boundary line points and the method of fitting the boundary line to the selected boundary points.

Outliers are extreme data values which appear to arise from a different process to most of the data. As a result they can cause bias and influence estimates of a statistical model. Outliers are of particular concern in boundary line analysis where the hypothesis is that the interesting biological relationship is expressed by the bounding observations of a response variable and a potentially-limiting factor. Despite the likely sensitivity of boundary line models to outliers, most of the reviewed articles did not indicate whether they removed outliers from datasets in their analysis. Of the 64 articles reviewed, only 14 indicated that they identified and removed outliers from their data. Of these 14, four articles did not indicate the criteria used to identify the outliers. A *neighbourhood density* procedure was used to identify outliers in two articles. In the neighbourhood density procedure, an observation is regarded as an outlier if it does not have at least some threshold number of neighbouring observations within a specified radius (Schnug et al., 1995). In one article the authors examined the scatter plot of y against x and identified points that looked unusual on the upper bound of dataset by '*inspection and judgement*'. One article used a bag plot to identify outliers. A *bagplot* is a two-dimension boxplot based on the measure of half-space depth (Rousseeuw et al., 1999). In five of the reviewed articles, outliers were identified on the *boxplot* of the response variable. However, it was not indicated the criteria used to define an outlier i.e. values of the upper and lower fences. A standardized objective method is needed to deal with outliers if boundary line analysis workflows are to be repeatable. Since boundary line models are applied to two variables with a joint bivariate distribution, the *bagplot* may provide a better tool for identifying outliers as it allows for joint distribution outliers to be identified in a dataset. Although the boxplot is commonly used, it is most suitable for univariate analysis as it takes no account of the value of the potentially limiting variable. The visual and neighbouring density methods are subjective as they involve arbitrary judgements or decisions e.g. the number of points and the size of neighbourhood is subjectively chosen, and so are not repeatable.

There are several approaches commonly used to select the boundary points and fit the boundary line in literature (Table S.2, Supplementary material). We have categorised them into two broad categories namely heuristic and statistical approaches. Heuristic approaches include the visual, binning, boundary line determination method (BOLIDES) and general quantile regression while the statistical approaches include Makowski quantile regression, stochastic frontier analysis, and the censored bivariate normal model methods. We describe these methods in detail in the following subsections. Another important considerations in boundary line analysis is the functional form of the boundary model. Various functional forms including linear (French and Schultz, 1984b), linear plateau (Andrade et al., 2023), trapezium (Nezamzade et al., 2020) and logistic regression (Fermont et al., 2009) models among others have been used in previous agronomic studies. Though the functional form is influenced by and should follow the upper boundary structure, it is recommended that the shape and parameters of the boundary line are assessed on the basis of their biophysical meaning (agronomic or physiological) (FAO and DWFI, 2015). If a boundary surface does not reflect that, it may raise concern as to whether the upper edges of the scatter actually represent the region of most efficient response.

4.2.1. Visual approach

This is a heuristic approach of boundary line fitting and is one of the simplest methods initially proposed by Webb (1972). A boundary line can be drawn along the largest data points which are simply identified by eye and the parameters of the fitted line can be obtained by the least square methods. Webb (1972) recognized the statistical difficulties that this method may bring as it has no means of accounting for measurement errors, measures of uncertainty, nor enabling reproducibility. Despite these weaknesses, this method has been applied in many studies involving yield gap analysis due to its simplicity (Abravan et al., 2016; Asten et al., 2003; Baral et al., 2022b,a; Dehkordi et al., 2020; French and Schultz, 1984b,a; Gorjizad et al., 2019; Haefele et al., 2003; Hajjarpoor et al., 2018; Mohammadi-Kashka et al., 2023; Nehbandani et al., 2020; Tagliapietra et al., 2018; Yousefian et al., 2021).

4.2.2. Binning approach

The binning approach is a heuristic approach that includes all variants of approaches that categorise the independent variable into ranges of values from which a single value of response variable is determined for each range and used to fit the boundary line (Fig. 6). For a scatter plot of yield against a factor x_i, x_i is divided into n number of sections (bins) and in each section, a boundary value corresponding to a set criteria, which can be the 90th, 95th, 99th or 99.7th percentile, is selected (Casanova et al., 1999; Kintché et al., 2017; Schmidt et al., 2000; van Vugt and Franke, 2018). An appropriate percentile value, is chosen so that it is not too high (e.g. 100th percentile) so as to remove the influence of outlier boundary points but also not too low to avoid cutting off influence larger response values (Schmidt et al., 2000). The selected boundary points (red solid symbols on Fig. 6) are used to fit the boundary line model.

Many authors have adopted this approach for yield gap analysis (Affholder et al., 2013; Casanova et al., 1999; Hoogmoed et al., 2018; Huang et al., 2008; Kintché et al., 2017; Li et al., 2017; Luo et al., 2020; Patrignani et al., 2014; Scarlato et al., 2017; Schmidt et al., 2000; Tasistro, 2012; van Vugt and Franke, 2018; Walworth et al., 1986). Similar to the visual method, this approach includes elements of subjectivity and does not account for measurement error, has no measure of uncertainty in the position of the boundary line and the model has no basis for checking for evidence of a boundary. Subjectivity arises in the selection of bin size and the selection of which quantile value to treat as a boundary point. There is currently no standardized method for bin size selection (Makowski et al., 2007; Milne et al., 2006a). The selection of different sizes of bins affects the number of points selected for fitting the boundary line and in turn, the position and parameters of the boundary line (Makowski et al., 2007).

Shatar and McBratney (2004) suggested a procedure to reduce the effect of arbitrary bin selection. They fix a moving window on the x-axis of the boundary plot of width 1/10 the range of x, then select a boundary value from successive increments of this window over the range. These selected values, a larger subset of the data than for other procedures, are then used to fit the model. Shatar and McBratney (2004) further suggested that measurement error could be accounted for through use of bootstrapping. Several boundary lines (say about 1000) are drawn by resampling and replacement of the data points in the dataset. The range of boundary lines drawn becomes the confidence interval of the boundary line. However, this method of determining the confidence interval is biased because the repeated replacement sampling from the same data results in a confidence interval always below the upper bounds of the dataset (Milne et al., 2006a).

4.2.3. BOLIDES approach

A third heuristic approach that has been commonly used in yield gap analysis (Bhattarai et al., 2017; Bucagu et al., 2014; Berrueta et al., 2020; Cao et al., 2019; Chen et al., 2018,2019; Fermont et al., 2009; Fu et al., 2021; Guo et al., 2021; Ndabamenye et al., 2013; Rhebergen et al., 2018; Silva et al., 2019; Wairegi et al., 2010; Wang et al., 2015; Zhang et al., 2019b, 2019, 2020) is the BOLIDES algorithm (Schnug et al., 1995). The dataset is first cleaned of outliers using a *neighbourhood density* procedure and then points are selected to which a boundary is fitted. The limitation of this method is that the minimum number of data points around a given point and the size of the neighbourhood is subjectively chosen. This affects the number of outliers in the data and ultimately, the position of the boundary line. There is currently no standard procedure for selecting the neighbourhood and the minimum number of neighbouring points.

The selection of the boundary points is done in a stepwise manner (Fig. 7a). Firstly, the minimum ($x_{\min}$), maximum ($x_{\max}$), and the maximum response point ($x_{y\max}$) values for the factor, x_i, in the dataset are identified. Starting with the largest response value at $x_{\min}$, the next boundary data point is the data point along the x-axis which encloses the dataset. Further boundary data points along the x-axis are identified until the boundary point equal to $x_{y\max}$ is reached. The boundary points between the $x_{\max}$ and $x_{y\max}$ are identified in a similar way starting from $x_{\max}$ but moving in the opposite direction. The selected points are then used to fit the boundary line and the parameters are extracted from it (Fig. 7b).

This approach, unlike the visual and binning approach, provides reproducible results if the same criteria are used to define outliers. However, it does not account for measurement error or uncertainty of the position of boundary line and does not provide any means of checking for evidence of the existence of a boundary in the dataset.

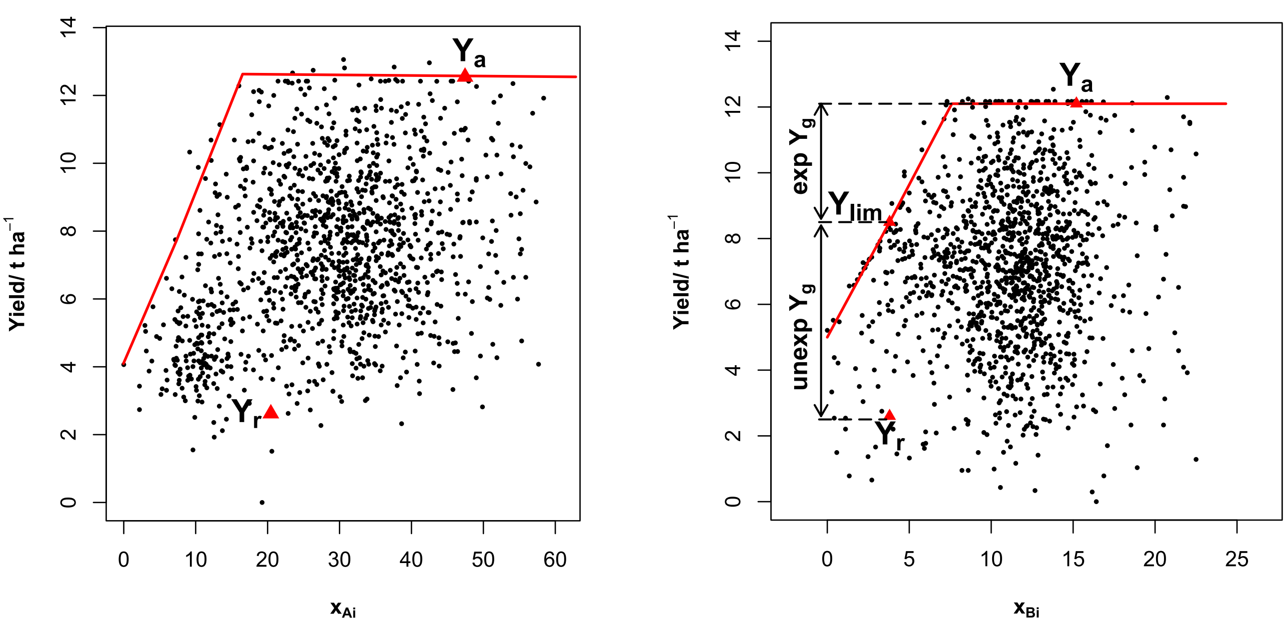
4.2.4. Quantile regression approach

Quantile regression models the τ^{th} quantile ($0 < \tau < 1$) of the prediction distribution. The τ^{th} quantile of a random variable Y can be defined as the value y for which the probability of obtaining values less than Y is greater or equal to τ. This concept can similarly be extended to linear regression such that the regression quantiles are estimated as conditional regression for different values of τ (Davino et al., 2014) as:

$$Q_Y(\tau|\mathbf{X}) = \mathbf{X}\boldsymbol{\beta}_\tau \tag{7}$$

where $\mathbf{Q_Y}(\tau|\mathbf{X})$ is a n x 1 vector of dependent variable Y conditional on τ, β is a $p \times 1$ vector of regression parameters, $\mathbf{X}$ is an $n \times p$ matrix of predictors. Estimates of the coefficients, $\mathbf{b}_\tau$, of β_τ are obtained by minimizing the weighted absolute residual values. The negative residuals are given weight equal to 1 - τ while the positive residuals are given weights equal to τ (Davino et al., 2014).

Quantile regression has been proposed as model for data in which the dependent variable responds in a complex way to interacting covariates. This is the case, for example, with the rate-limiting form of the law of the optimum presented in Equation (2). Under the model, the form of the response of the dependent variable to one covariate can vary, expressed in different functional forms for quantiles of the prediction distribution. Therefore, some upper regression quantile can be regarded as a boundary line and modelled as the quantile regression for some τ (e.g. Baudron et al. 2019 used the 90th percentile (See Box 3) while Wang et al. 2022 used the 95th percentile). The percentile value used to represent the boundary line is typically chosen so that it is not too low to include points that are affected by other unmeasured limiting factors but also not too high to be affected by measurement error (Schmidt et al., 2000). There is however, no inference that can be made to ascertain whether the selected quantile function can be regarded as a boundary. The quantile regression method has been applied in yield gap analysis studies using boundary lines (Edreira et al., 2017; Fink et al., 2022; Grassini et al., 2009; Lollato et al., 2017; Neuhaus and Sadras, 2018; Rizzo et al., 2021; Sadras and Angus, 2006).

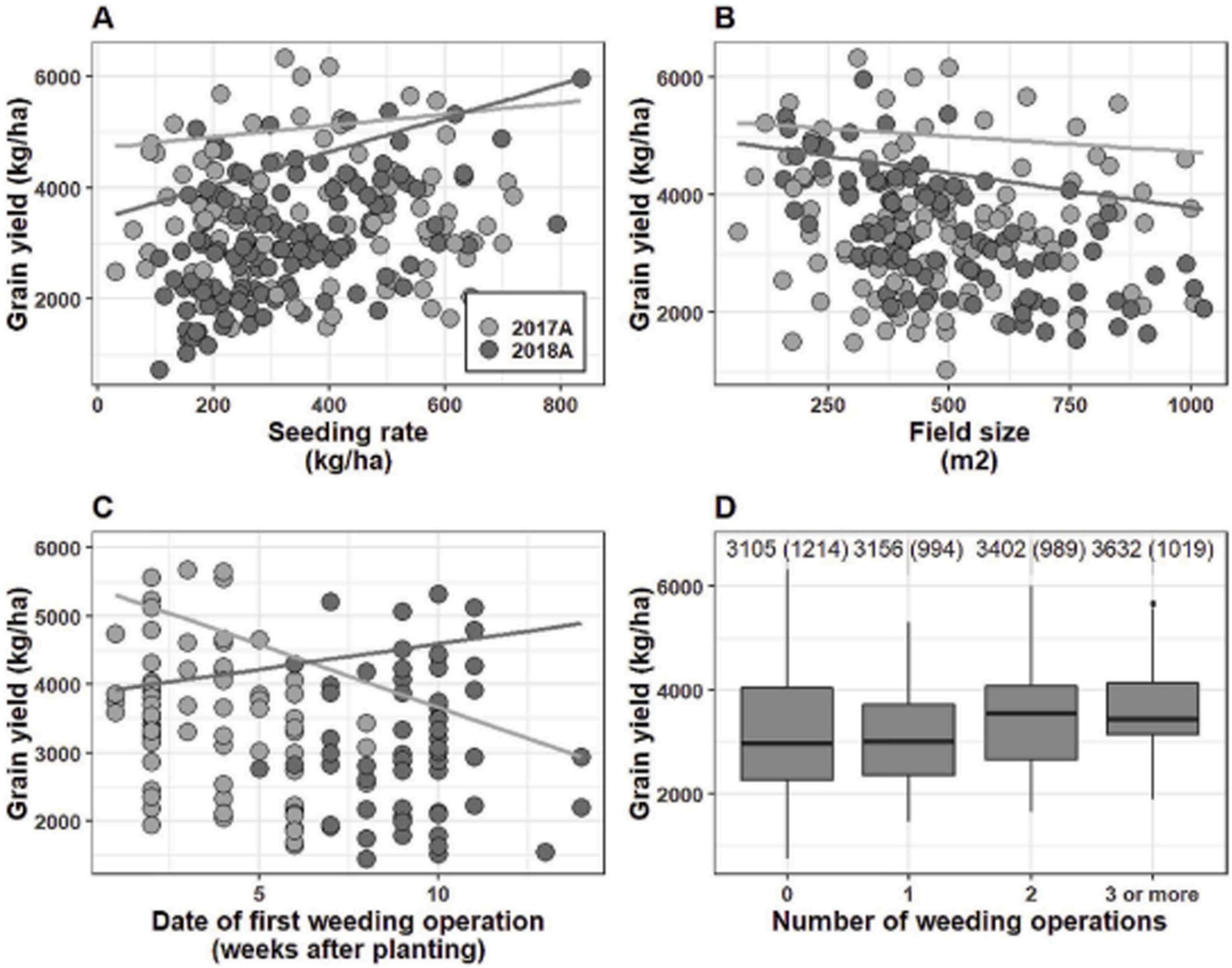


(a) (b)

Fig. 5. Decomposition of yield gaps into explained (exp Y_g) and unexplained (unexp Y_g) yield gaps when only two factors, A and B, are considered. *Yr* is actual yields of farm, *Ya* is the attainable yield and *Ylim* is the yield predicted by most limiting factor.

Box 3: How to increase the productivity and profitability of smallholder rainfed wheat in the Eastern African highlands? Northern Rwanda as a case study (Baudron et al., 2019).

Baudron et al. (2019) studied how different factors affect wheat yield in Rwanda with an aim of finding ways of increasing productivity. They used multivariate stochastic frontier analysis in combination with univariate boundary line analysis for this purpose. The factors which were found to significantly affect yield gap were identified by the stochastic frontier analysis and were further evaluated using the boundary line analysis to gain further insight into how they affect yield. Factors including seeding rate, farm size and date of first weed were subjected to boundary line analysis using quantile regression method with the 90th percentile used as the boundary line as shown in Box-Fig. 4.



Box-Fig 4. Wheat grain yield as a function of (A) seeding rate; (B) field size; and (C) date of the first weeding operation; and (D) wheat grain yield as a function of the number of weeding operations. In (A), (B) and (C), the light grey lines and the dark grey lines represent the linear regressions fitted through the 90th percentile of the season 2017A data and the 2018A data, respectively. In (D), means are given for each category, followed by the standard deviation in parentheses.

The positive effect of seeding rate on wheat grain yield during the season 2018A (obtained From SFA) was confirmed by the increasing boundary lines in the univariate boundary line analysis. Similarly, the negative effect of field size on wheat grain yield was confirmed by the decreasing boundary lines. The boundary line was also found to decrease when considering time between planting and the first weeding operation as the independent variable during the season 2017A. Boundary lines in this case provide a tool for studying how the different factors affect the yield and how they can be improved to increase productivity.

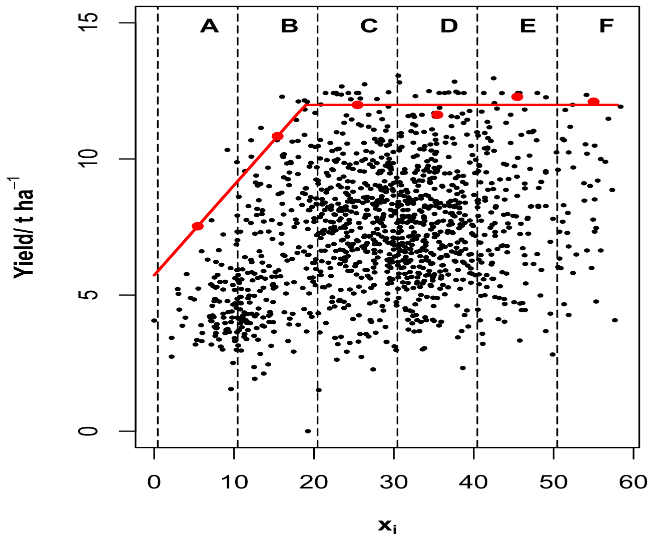


Fig. 6. The process of fitting the boundary line using the binning approach with fixed, non-overlapping bins. Factor x_i is divided into sections A, B, C, D, E and F separated by dashed vertical lines. The red solid symbols, representing the boundary point of each section, are selected as the 95th percentile of the data in each section. The red line is the fitted boundary line model to the selected points.

When the targeted quantile value which corresponds to the boundary line function is known, quantile regression provides a good basis for deriving the boundary line as it uses all the data points in a dataset without the bias of removing or selecting a subset of data points or making arbitrary bins (Makowski et al., 2007). However, the suitable quantile value is usually not chosen objectively and therefore, this method is classified as heuristic. Without an objective method of choosing the quantile value, reproducibility is a challenge. In a recent study, Andrade et al. (2023) used a Bayesian approach called Bayesian segmented quantile regression (BSQR) to fit the boundary lines and determine various critical soil nutrient values in vineyard soils for fertilizer recommendations. They found that the BSQR model was highly sensitive to quantile selection which can directly affect parameter estimates of the boundary line and subsequent critical levels, and sufficiency ranges for nutrients in soils. This sensitivity may lead to variations in the estimated nutrient critical values, potentially affecting the accuracy of fertilization recommendations. This highlights the need for a more objective method for quantile selection. Furthermore, this method does not have any mechanism to test for the presence of an upper boundary.

4.2.5. Makowski quantile regression method

The Makowski quantile regression approach is a development of the general quantile regression approach described in Section 4.2.4. The lack of an objective method to decide on the quantile value (τ) for the quantile regression approach is the main challenge of the general quantile regression. Makowski et al. (2007) proposed a method to determine of the appropriate quantile value (τ) statistically from the distributions of measurement error of yield and the limiting factor, using some expert assumptions and judgments. Makowski et al. (2007) propose that the distribution of the measurement error and the limiting factor can be assumed by agronomists and statisticians based on previous studies or expert knowledge. The challenge for using this model is that in most cases where the boundary line method is used for yield gap analysis, data are gathered from surveys or different non-experimental plots without replicate measurements making it difficult to eliminate the measurement errors. In addition to this, the distribution of the limiting factor(s) is also difficult to estimate as it is unknown in reality

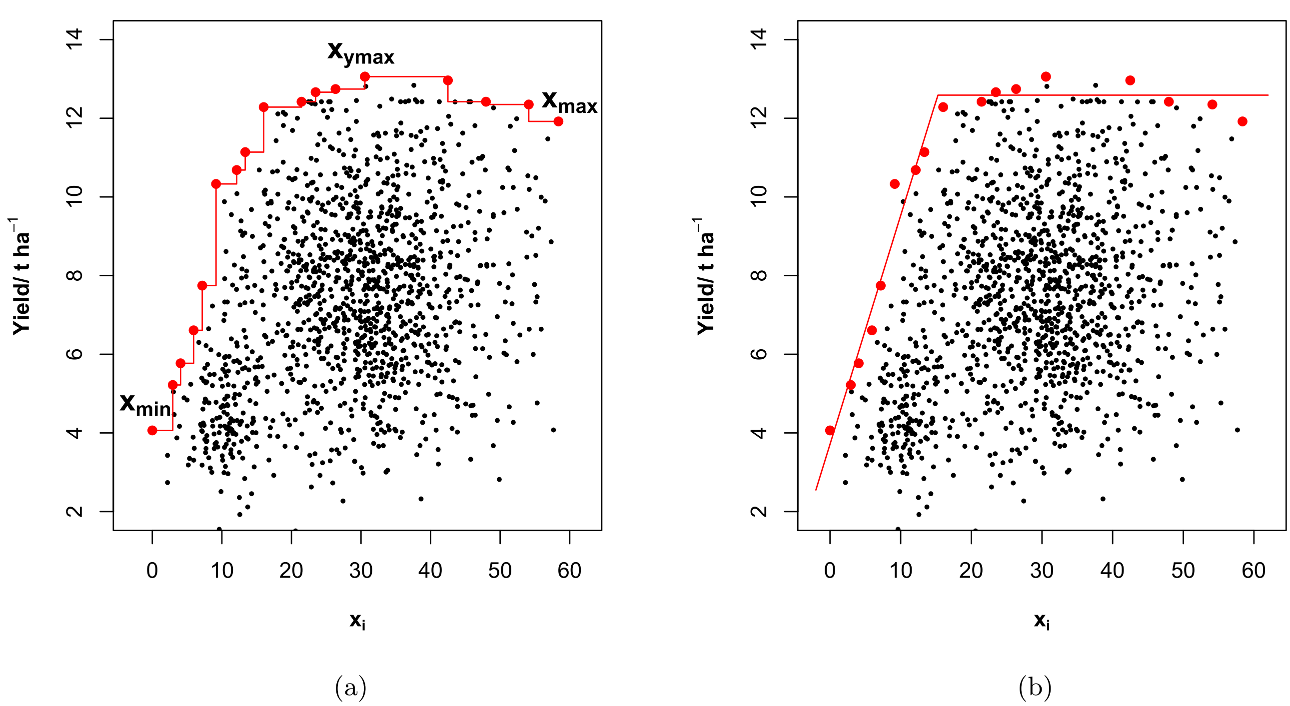


Fig. 7. (a) Process of selecting boundary points using BOLIDES. x_{ymax} is the value of the factor corresponding to the maximum yield, x_{min} corresponds to the largest yield at the smallest value of factor in dataset and x_{max} corresponds to the largest yield at the largest value of factor in dataset. The red dots represents the selected boundary points by implementing BOLIDES (b) The boundary line fitted to the selected points using a broken stick model.

thereby making the estimation of the quantile value very difficult to achieve practically as a lot of information is needed to make the assumptions of the error distribution and the limiting factor distribution. Therefore, significant further work is needed before this can be considered a working method.

4.2.6. Censored bivariate normal model

The censored model approach for setting out the boundary line developed by Milne et al. (2006a), is categorised as a statistical approach as it uses explicit statistical assumptions to set out the boundary line and estimate its parameters. It is based on the principle of a censored bivariate distribution. Parameters comprise the parameters of the bivariate distribution (the mean of the response variable (μ_y), mean of the independent variable (μ_x), the variance of the response variable (σ_y), the variance of the independent variable (σ_x), and correlation (ρ)), the parameters of the boundary lines which acts as the censor of the bivariate model and the measurement error of the response variable. The parameters of the boundary line depend on the chosen model (i.e. linear, polynomial, etc.) as well as the parameter that describes the error of the boundary line (see Box 4 and 5). The model parameters are estimated using the maximum likelihood approach given the available data (Milne et al., 2006a). The likelihood in simple terms will be the best combination of unknown parameters that could have likely produced the available dataset. Therefore, the combination of parameters with the highest likelihood is most likely to have produced the available data. The suitability of the derived model can be tested by comparing it with a simple uncensored bivariate model (null model) using Akaike's information criterion (AIC). The AIC imposes a penalty for additional parameters when comparing with a simple model. If an additional parameter does not improve the model significantly, it is better to use the simple model (null model).

Box 4: Theory of the censored bivariate normal model (Lark and Milne, 2016)

A censored bivariate normal distribution for which the boundary line acts as the upper censor can be described by the function:

$$f(y, x) = \phi(\boldsymbol{Z}|\boldsymbol{\mu}, \boldsymbol{C}) \tag{8}$$

where ϕ represents the bivariate normal density function with means $\boldsymbol{\mu}$ and covariance matrix $\boldsymbol{C}$, and the vector $\boldsymbol{Z}$ represents the censor function with parameters, $\boldsymbol{\beta}$. Given a boundary model, $b(x) = \overline{y}$, is the censor, a variate {y, x} for which $y > \overline{y}$ is replaced by variate $\{\overline{y}, x\}$. As the variable y is measured with error, $N(\overline{y}, \sigma_e)$, and so observations above the censor are only due to measurement error, the variate $\{y, x\}$ can be written as $\{\widetilde{y}, x\}$ to show influence of measurement error. The censored bivariate normal model can be written as a function of three sets of parameters, the censoring parameter, $\boldsymbol{\beta}$ (which represents the boundary line), the parameters of the bivariate random normal distribution (means, $\boldsymbol{\mu}$, and (co)-variance, $\boldsymbol{C}$) and the measurement error, σ_e, of response variable y.

$$f(\widetilde{y}, x|\boldsymbol{\beta}, \boldsymbol{\mu}, \boldsymbol{C}, \sigma_e) \tag{9}$$

To keep things brief, the parameters from the density functions can be dropped. Following the properties of conditional densities, the function $f(\overline{y}, x)$ can be written as

$$f(\widetilde{y}, x) = f(\widetilde{y}|x)f(x) \tag{10}$$

where $f(x)$ is the probability density function of x. Assuming x is measured without error, as in the general linear model, the conditional density in Equation (10), can be written as a convolution ($f*g$) of the two functions as

$$f(\widetilde{y}, x) = f(\overline{y}|x) * f_N(v|0, \sigma_e) \tag{11}$$

The conditional density $f(\overline{y}|x)$ in Equation (11) is the censoring of the conditional density $f(y|x)$ and can, therefore, be written as

$$f_N(y|\mu_{y|x}, \sigma_{y|x}) \tag{12}$$

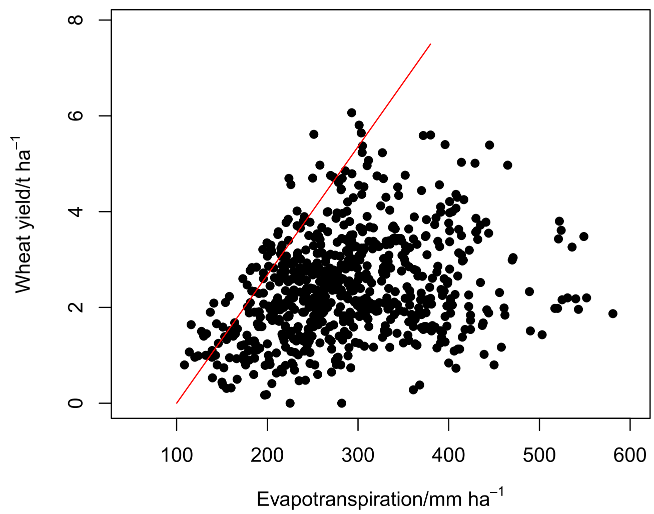
where $\mu_{y|x}$ and $\sigma_{y|x}$ are the conditional mean and standard deviation, respectively, of y. The censored conditional density as a right-censored distribution (upper boundary), can be therefore, be broken down as

$$f(\overline{y}|x) = \begin{cases} f_N(y|\mu_{y|x}, \sigma_{y|x}) & \text{if } y < b(x), \\ \int_{b(x)}^{\infty} f_N(y|\mu_{y|x}, \sigma_{y|x})dy & \text{if } y = b(x), \\ 0 & \text{if } y < b(x) \end{cases} \tag{13}$$

For some proposed set of parameters, $\boldsymbol{\beta}$, $\boldsymbol{\mu}$, $\boldsymbol{C}$ and σ_e and a pair of observed values, $\widetilde{y}$ and x, the density can be computed using Equation (13) and therefore, the likelihood given the observations. It can be seen that if there are more observations at the boundary, given the measurement error, the likelihood will be larger. The observations above the boundary line have zero density values hence do not contribute to the likelihood value.

Box 5: Yield gap analysis using the bivariate censored method (FAO and DWFI, 2015)

Data for the actual wheat yield and estimated evapotranspiration in China, Mediterranean Europe, North America, and Australia was collected. The boundary line was fitted using the bivariate censored model of Milne et al. (2006a). In this particular case a linear boundary line model, $y = ax + b$ was assumed and its parameters were estimated using the maximum likelihood approach. The estimated parameter values were $a = 0.025$ with 95 percent confidence interval (0.020, 0.030) and $b = -2.458$ with 95 percent confidence interval ($-3.412, -1.504$). The variation around the boundary, $\sigma_B = 0.971$, with confidence interval (0.791, 1.151). The suitability of the model was checked using AIC and the boundary line model was found to describe the data better than the null model which was assumed to be the bivariate normal model Box-Fig. 5.



Box-Fig 5. Relationship between estimated evapotranspiration and wheat yield (FAO and DWFI, 2015).

The strength of this approach is that it has explicit statistical assumptions and eliminates the subjectivity. Unlike the heuristic approach, all the data points are used in this approach which is consistent with statistical principles that guard against deliberate or undeliberate removal of data in a datasets. This approach ensures that reproducibility of the boundary line is achieved, accounts for observational errors and the uncertainty of the boundary line position can be derived. Unlike the methods that use the bootstrapping approach, the confidence interval is not limited by the upper bound of the data points. The actual value of the measurement error parameter may not always be available. In such cases, other methods to estimate the measurement error parameter have been used including the use of the nugget variance for a variogram of the response variable (Lark et al., 2020), use of profile likelihood of measurement error (Lark and Milne, 2016) or finding the maximum likelihood estimate along with the other model parameters (Kindred et al., 2015).

4.2.7. *Stochastic frontier approach*

Stochastic frontier analysis (SFA) is a statistical method of economic modelling which has been used in production ecology to fit the upper limit of a response variable given an independent variable(s). It has been applied in yield gap analysis studies in recent studies (Baudron et al., 2019; Dossou-Yovo et al., 2020; Silva et al., 2017b, 2019, 2021). The frontier model describes the maximum output that can be achieved given a level of input(s). Any point below this frontier is a result of a composite error that is made up of the sum inefficiency and random error of measurement as shown in the stochastic frontier equation (14). This is normally expressed in log form

$$\log(Y_r) = \log(f(x_i|\beta) + \epsilon_i) - u_i \tag{14}$$

where $f(x_i|\beta)$ is the frontier model, ϵ is a random error term and u_i, the inefficiency is a positively valued random variable which expresses the effect of factors which reduce the output below the frontier response-equivalent to the efficiency gap described above. Technical efficiency in SFA is defined as the ratio of the observed output, Y_r here, to the term $f(x_i|\beta) + \epsilon$ (Silva et al., 2017a). From equation (14) it follows that

$$\begin{aligned} -u_i &= \log\left(\frac{Y_r}{f(x_i|\beta) + \epsilon}\right) \\ &= \log(E_T) \end{aligned} \tag{15}$$

and so

$$E_T = e^{-u_i} \tag{16}$$

It is assumed that the error term ϵ is normal with zero mean and that u_i is a non-negative number with an exponential or gamma distribution or some truncated distribution such as the half normal with mean $z_i v$ and variance σ^2. The latter distribution is commonly preferred (Aigner et al., 1977). The factors that affect inefficiency can further be modelled as

$$u_i = \mathbf{Z}_i^T \mathbf{V} + w_i \tag{17}$$

where z_i is a vector of explanatory variables associated with inefficiency and v is a vector of unknown coefficients and w_i is a random variable. The unknown parameters in equations (14) and (17) can be estimated simultaneously by maximum likelihood. Besides the maximum likelihood approach, other methods like the corrected ordinary least square, generalized method of moments and Bayesian methods have been used in econometrics. The Bayesian methodology has potential to improve the robustness of modelling, particularly from small datasets, if robust and important prior distributions are available for parameters.

The advantages of SFA are that it is objective and reproducible, uses all the data points, and can account for measurement errors. In addition, this method allows the input of multiple factors to model their simultaneous effect on a response variable. This provides the additional capability of studying yield gaps at farm level rather than just at crop

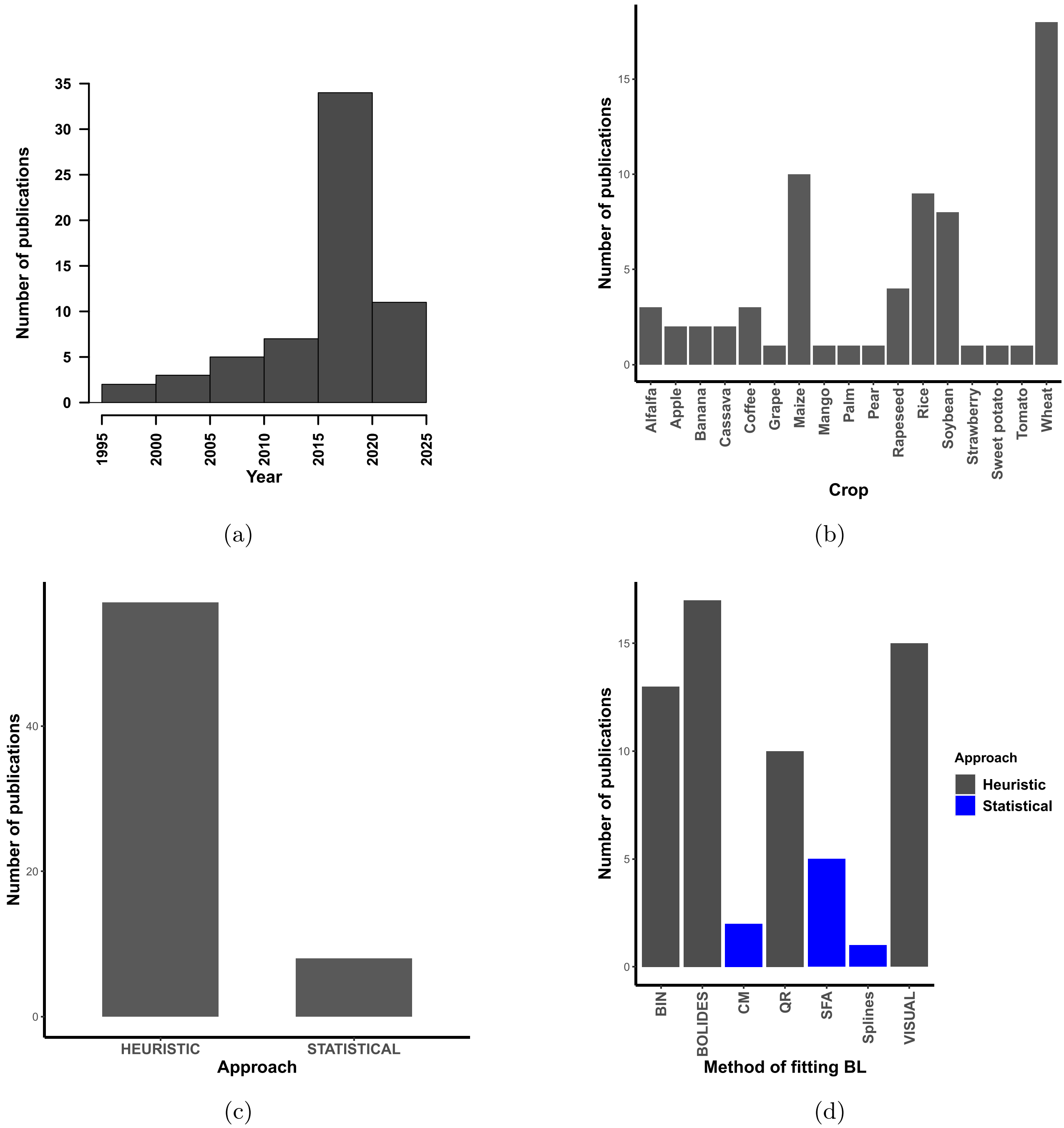


Fig. 8. Number of articles published during the last 28 years (1995–2023) that have utilised the boundary line (BL) approach for yield gap analysis (a), Crops that have been studied (b) and the number of publications that used the different approaches (c) and boundary line fitting methods (d). CM represents the censored model, QR is quantile regression and SFA is the stochastic frontier analysis.

level (Silva et al., 2017b). For example, labour at farm level is distributed amongst different enterprises, therefore, labour can be inputed as an input in the SFA for a crop of interest to determine whether it is the cause of the observed inefficiency (Silva et al., 2017b, 2019). This can help to restructure labour provisions to achieve efficiency at farm level.

5. Trends in the usage of various boundary line fitting approach

There has been an increase in the use of boundary line methodology for yield gap analysis over the past two decades (Fig. 8a). This indicates its importance as a method for yield gap analysis and therefore, the need to standardise the methodology for better interpretation and comparison amongst studies. A variety of crops (alfalfa, apple, banana,cassava,coffee, grape, maize, mango, palm, pear, rapeseed, rice, soybean, sweet potato, tomato and wheat) have been studied using this methodology in different regions of the world (Casanova et al., 1999; Cossani and Sadras, 2018; Fermont et al., 2009; Hajjarpoor et al., 2018; Kintché et al., 2017; Lark et al., 2020; Shatar and McBratney, 2004; Silva et al., 2019; van Vugt and Franke, 2018) with cereals (maize, wheat and rice) accounting for over 50% of the studies (Fig. 8b), Soybean was studied in about 12% of the studies while the rest of the crops accounted for less than 7% each. Different boundary line fitting methods are available and have been used in these studies. The question arises, which approach of fitting the boundary line should one use? Although the statistical methods provide a more reproducible analysis and allow quantification of uncertainty of the boundary line position, few studies have used them in general (e.g. Kindred et al., 2015; Lark and Milne, 2016; Lark et al., 2020). More recent studies for yield gap analysis have continued to use the heuristic approaches because of their simplicity to execute (e.g. Gorjizad et al., 2019; Hajjarpoor et al., 2018; Nezamzade et al., 2020).

Of the peer-reviewed articles that were selected during the search for this review (n = 64), 58 used a heuristic approach for fitting boundary lines while only 8 used the statistical approach (two studies combined two methods) (Fig. 8c). BOLIDES was the most commonly used method, 18 studies, while the binning, visual and the quantile regression methods were used in 13, 15 and 10 studies respectively (Fig. 8d). The statistical methods, censored model and SFA were used in two and five studies respectively. Two studies (Duan et al., 2022; Wairegi et al., 2018) did not clearly indicate which method they used. One study fitted the boundary line using splines (Niang et al., 2017). It is not known whether there are systematic and important differences in the outcome of the boundary line analysis if statistical rather than heuristic approaches are used or when different statistical approaches are used. There is, therefore, a need for comparative studies to examine the differences and to assess their practical importance. The choice of a method to set out the boundary line for use in yield gap analysis may depend on various factors. These may include the objective of the study, usability (simplicity/complexity) and availability of the method, and the amount of data available.

The researcher's objective is an important determinant of the approach which is used. Many authors have concluded that the boundary line is most useful for checking the relative importance of factors in yield gap analysis (Shatar and McBratney, 2004; Silva et al., 2019). However, boundary line analysis allows us to draw stronger quantitative conclusions. An example is the use of the boundary line to verify some standard nutrient guidelines. Evanylo et al. (1987) used the boundary line approach to determine the soil critical values of Ca, P, K and Mg for soyabean on fine and coarse textured soils. Similarly, Lark et al. (2020) used the statistical censored model method for fitting boundary line to check if the model outcomes were consistent with RB209 index values for P, K and Mg requirements for wheat production in the soils of the United Kingdom. Furthermore, they compared boundary lines for available phosphorus for different subsets defined on pH to check its effect on the boundary line parameters. A similar study by Andrade et al. (2023) used boundary line methodology to obtaining reference values for nutrients in vineyard soils. These kind of studies may require precise parameter estimation with confidence intervals so statistical rather than heuristic approaches may be advantageous. The use of Bayesian statistical methods such as the BSQR proposed by Andrade et al. (2023) as well as the censored bivariate normal model by (Milne et al., 2006b) provide ability to attach uncertainty to the boundary line parameters if all other bottlenecks to their use are resolved. The censored bivariate normal model can surely benefit from application of Bayesian approaches to estimate the measurement error value which is an input but rarely available in most datasets.

The usability of a method is another determining factor of which approach to use. Though statistical approaches provide more robustness than heuristic approaches, they may be more complex to use which may make it difficult for researchers with a limited statistical background (Harris and Smith, 2009). As an example, the censored model method of Milne et al. (2006a) requires initial parameter values which may provide a challenge for agronomists with limited statistical experience especially when the boundary line model is non-linear. Another statistical approach, the quantile regression of Makowski et al. (2007), has not been developed into a full working method as it requires some strong assumptions about the distribution of the errors and limiting factor(s). It is, therefore, vital to come up with interactive tools that help the end-users (researchers or agronomists in this case) utilise and make good interpretations if statistical methods are to be fully utilised. For instance, many studies (Gorjizad et al., 2019; Hajjarpoor et al., 2018; Nehbandani et al., 2020; Nezamzade et al., 2020) have used the visual method, a heuristic approach, for fitting boundary line despite recognising the availability of statistical approaches like the censored model of Milne et al. (2006a) and quantile regression of Makowski et al. (2007) citing simplicity as the reason for selecting the visual method. The BOLIDES has also been widely used maybe because it is easier to follow and probably because of the availability of a software that executes the process.

The amount of data available is another factor that is vital in the choice of method to use for boundary line fitting and may render some methods suitable or unsuitable. While the heuristic methods can be easily executed with relatively fewer data available, some statistical approaches may result in the poor fitting of a boundary line. Approaches that utilise the maximum likelihood method in parameter estimation (e.g. censored model and stochastic frontier analysis) require that there is sufficient amounts of data available as its outcome is dependent on the observations in the dataset (Myung, 2003). Without sufficient data these methods will not converge on a suitable boundary. Although the heuristic methods can easily be implemented using a smaller datasets, it does not make them better than statistical methods in these cases. The use of Bayesian methods can help overcome the challenge of less data availability as it uses some prior knowledge and this is vital in cases where there is limited data. Bayesian approaches have not been fully utilised for yield gap analysis despite their ability to resolve the challenge of lack of sufficient data. Though the addition of the expert opinion and knowledge may enhance the results of the model, there is a need to be cautious when including expert opinion in models as this may lead to unsatisfactory results if poorly implemented. Expert information may contain personal biases and preferences that reduce its objectivity and reliability. Data on qualitative factors (e.g. crop variety and manure type among others) have not been incorporated into yield gap analysis using boundary lines (see Table S.2) except when SFA has been applied (Baudron et al., 2019; Silva et al., 2017b,a). However, these are important determinants of yield gaps along with quantitative factors. Further research is required to enable the addition of qualitative factors in the yield gap process using boundary lines. This may be a challenge for statistical approaches like the censored model of Milne et al. (2006a) which works on the assumption the data follows a bivariate normal distribution.

It is also important to note that the choice between the statistical and heuristic approaches may affect the conclusion of yield gap analysis using boundary lines when interpreted as the law of the minimum. When statistical methods, which allow for the computation of confidence interval of the boundary line, are used, boundary lines with confidence intervals that do not overlap can be concluded to be different and the boundary line that predicts the minimum response can easily be identified. However, if the confidence intervals of boundary lines are overlapping, further statistics are needed to check which boundary line predicts the minimum response. This is not possible when heuristic methods are used. Studies that interpreted the boundary line as the law of the minimum while utilising the heuristic approaches in setting out the boundary line (e.g. Casanova et al., 1999; Wairegi et al., 2010), may have different outcomes if statistical approach which account for confidence interval of boundary lines were used.

6. Conclusion

The methods for fitting boundary lines for yield gap analysis have been identified with the heusteric methods being commonly used (89%). The selection of boundary line fitting method has been identified to be affected by different factors that include the objective of the study, the usability of the method (simplicity/complexity) and data availability. The heuristic methods are often simpler to use and this is likely to be the reason they are more commonly adopted. However, the statistical methods provide a more robust approach despite being more complex. It is, therefore, important that interactive tools are developed that can help facilitate the use of statistical methods by researchers and agronomists. A second issue with statistical methods, especially those based on the maximum likelihood, is that they require large amounts of data to converge. The use of Bayesian statistics provide a solution for this data availability challenge because it incorporates prior knowledge of distributions in its implementation. Nonetheless, there is a gap in knowledge on how the statistical and heuristic methods of setting out the boundary line compare (as well as how different statistical methods compare), if there are important systematic differences, and how they affect outcome of the yield gap analysis and its interpretation. We therefore, recommend a comparative study using various data sets is needed to explore the strengths and weaknesses of statistical and heuristic methods. Further, there is a lack of exploratory tools in the boundary line framework that evaluate evidence of bounding effects in a plot despite it being a vital initial step for boundary line modelling.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

No data was used for the research described in the article.

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Appendix A. Supporting information

Supplementary data associated with this article can be found in the online version at doi:10.1016/j.fcr.2024.109365.

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