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MIXED EFFECTS AND SEMI-PARAMETRIC BAYESIAN INTEGRATION MODELS FOR MEASUREMENT ERROR CORRECTION IN THE CONTEXT OF FERTILIZER APPLICATION LEVELS: A SIMULATION STUDY

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Abstract: In agricultural research, the precision of variable measurement is crucial as it forms the foundation for accurate estimations and informed decision-making. However, the presence of measurement errors in real-world data often leads to skewed estimates and flawed conclusions. This study addresses the common challenge of measurement error, focusing on the optimization of fertilizer application levels—a critical factor in sustainable agriculture. Through carefully designed simulation studies, we introduce controlled measurement errors into Gaussian process models and rigorously evaluate their effects on regression outcomes. To strengthen the reliability of our findings, we integrate mixed effects models with a semi-parametric Bayesian framework, leveraging the MCMC Gibbs Sampler for robust inference. Our results highlight the significant impact of measurement errors on the precision of regression estimates, while also demonstrating that advanced statistical models—particularly those combining mixed effects with Bayesian integration—can effectively reduce these errors. This research not only improves the accuracy of agricultural analyses but also offers practical methodologies for optimizing fertilizer use, ultimately contributing to increased agricultural productivity and sustainability. The implications of our findings

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extend beyond theoretical significance, providing actionable insights that can transform resource management in agricultural practices.

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1. INTRODUCTION

Accurate measurement of variables is paramount in statistical modeling, particularly in agricultural research where precise estimations drive informed decision-making processes [1,2,3]. However, real-world data often suffer from measurement errors, which can lead to biased estimates and erroneous conclusions [4,5]. Addressing this challenge requires robust methodologies capable of correcting for measurement errors and ensuring the reliability of regression analyses.

This research focuses on correcting measurement error models and optimizing fertilizer application levels through simulation studies, with a specific emphasis on land size area and various covariates including soil characteristics, fertility, and moisture content. The study simulates data from variants of Gaussian processes, allowing for controlled manipulation of measurement errors within the regressors [6].

The primary objective of this simulation study is to evaluate the impact of measurement errors on independent variables (regressors) in regression analysis. By introducing controlled measurement errors into the regressors, the study aims to assess how these errors influence the accuracy and coverage of estimates provided by the regression model [7,8].

Understanding the effects of measurement errors on regression outcomes is crucial for improving the reliability and applicability of statistical models in agricultural research [9,10,11,12]. By identifying and mitigating the impact of measurement errors, researchers can enhance the accuracy of predictions and optimize fertilizer application levels, thereby contributing to more efficient and sustainable agricultural practices [13,14,15,16].

In this paper, we present the methodology employed in the simulation study, discussing the implications of measurement errors on regression estimates and highlighting the importance of corrective measures in enhancing the reliability of statistical analyses in agricultural research [17,9,18]. Additionally, we integrate mixed effect models to account for the hierarchical structure of the data, further enhancing the robustness of our analyses [19,20]. Then incorporate the Semi-Parametric Bayesian integration approach through the Gibbs Sampler, Markov Chain, Monte Carlo [21]. The findings from this research have significant implications for optimizing agricultural practices and improving productivity while minimizing resource wastage.

2. METHODOLOGY

Linear Regression Model with Measurement Error:

Consider the linear regression model with measurement error:

$$y_i = \beta_0 + \beta_1 X_i^* + \varepsilon$$

where X_i^* is the observed independent variable with measurement error.

It can be represented as: $X_i^* = X_i + \eta_i$

Our goal is to find the bias in the estimate of β_1 due to the measurement error η .

Therefore,

We start with the model:

$$Y_i = \beta_0 + \beta_1 (X_i + \eta_i) + \varepsilon$$
$$Y_i = \beta_0 + \beta_1 X_i + \beta_1 \eta_i + \varepsilon$$

Now, we can take the expectation

$$E(Y_i) = \beta_0 + \beta_1 X_i + E(\beta_1 \eta_i) + E(\varepsilon_i)$$
$$E(Y_i) = \beta_0 + \beta_1 X_i + \beta_1 E \eta_i + E(\varepsilon_i)$$

Given that $E(\varepsilon_i) = 0$ and $E(\eta_i) = 0$

We have:

 $\mathrm{E}(Y_i) = \beta_0 + \beta_1 X_i$

This shows that the expectation of *Y* is linearly related to *X* without bias. However, the coefficient β_1 in our model represents the impact of X^* on *Y*, not *X*.

So, let's find the expectation of Y_i conditioned on X_i :

$$E(Y_i | X_i) = \beta_0 + \beta_1 X_i + \beta_1 E(\eta_i | X_i) + E(\varepsilon_i)$$

Given that $E(\varepsilon_i) = 0$ and $E(\eta_i) = 0$ (Since η is assumed to be independent of X,

We have

$$\mathrm{E}(Y_i \mid X_i) = \beta_0 + \beta_1 X_i$$

This implies that X_i^* on average has the same effect on Y_i as X_i meaning there is no bias in estimating β_1 .

2.1 Linear Mixed Effects Models:

Mixed effects models extend the standard linear regression model to incorporate both fixed and random effects.

Mathematically, the mixed effects model can be represented as:

$$Y_i = \beta_0 + \beta_1 X_i^* + \gamma_{0j} + \gamma_{1j} X_i + \varepsilon_i$$

Where:

- γ_0 and γ_1 represent the random intercept and slope for the j^{th} group or levels.
- ε_i is the error term for the i^{th} observation.

In mixed effects models, the random effects account for the hierarchical structure of the data, capturing variability within groups or levels. This enhances the robustness of the analysis and provides more accurate estimates of regression coefficients.

2.2 Non Linear Regression Model with Measurement Error

Consider the non-linear regression model with measurement error: $Y_i = f(X_i^*, \beta) + \varepsilon_i$

Where X_i^* is the observed independent variable with measurement error and f is a non-linear function of X_i^* with parameters β .

Similar to before, X_i^* can be represented as $X_i^* = X_i + \eta_i$

Our goal is to find the bias in the estimate of the parameters β due to the measurement error η . Therefore, we can start the model:

$$Y_i = f(X_i + \eta_i, \beta) + \varepsilon_i$$

We can use the Taylor expansion to approximate $f(X_i + \eta_i, \beta)$ around X_i as:

$$f(X_i + \eta_i, \beta) \approx f(X_i, \beta) + f'(X_i, \beta)\eta_i$$

Substituting this approximation into the model, we get:

$$Y_i \approx f(X_i + \eta_i, \beta) + f'(X_i, \beta)\eta_i + \varepsilon_i$$

Now, let's take expectations:

$$E(Y_i) \approx E(f(X_i + \eta_i, \beta)) + E(f'(X_i, \beta)\eta_i) + E(\varepsilon_i)$$

Given that $E(\varepsilon_i) = 0$ and $E(\eta_i) = 0$,

We have:

$$E(Y_i) \approx E(f(X_i, \beta))$$

This shows that the expectation of Y related to X through the non-linear function f without

bias. However, estimating parameters β using X_i^* can introduce bias due to the measurement error.

2.3 Non-linear Mixed Effects Models

Mixed effects models can also be extended to non-linear regression settings. These models incorporate both fixed and random effects while allowing for no-linear relationships between the variables. The structure of the mixed effects model in the non-linear case would be similar to the linear case but function f may be non-linear.

$$Y_i = f(X_i, \beta) + \gamma_{0i} + \varepsilon_i$$

Where:

- γ_{0i} Represents the random effect for the j^{th} group or levels.
- ε_i Is the error term for the i^{th} observation.

Incorporating random effects into the non-linear mixed effects model accounts for the hierarchical structure of the data, providing more accurate estimates of the parameters $\beta\beta$ and capturing variability within groups or levels.

2.4 Root Mean Square Error (RMSE)

The Root Mean Square Error (RMSE) is a widely used metric for assessing the accuracy of a predictive model. Its formula is:

$$RMSE = \sqrt{\frac{\sum_{i=i}^{n} (y_i - \hat{y}_i)^2}{n}}$$

Where:

- y_i Represents the observed values of the dependent variable.
- \hat{y}_i Represents the predicted values of the dependent variable by the model.
- *n* is the total number of observations.

2.5 Deviance Information Criterion (DIC)

The DIC is a measure used in Bayesian statistics to compare and select between different Bayesian models. The equation for DIC is:

$$DIC = D(\theta) + 2pD$$

Where:

 $D(\theta)$ = the mean deviance of the posterior distribution of the parameters θ

pD = effective number of parameters, which is calculated as

Here, $D(\theta)$ is the deviance of a particular model, which is calculated as:

$$D(\theta) = -2\sum_{i=1}^{n} \log(P(y_i \mid \theta))$$

Where: $P(y_i | \theta)$ is the likelihood of the observed data y_i given the parameters.

4. RESULTS AND FINDINGS

Data were simulated from variants of the following Gaussian process:

$$y_i = \beta_0 + \beta_1 x_{1i}^* + \beta_{2i}^* + \beta_{3i}^* + \beta_{4i}^* + \varepsilon$$
$$x_i^* = x_i + \mu_i$$
$$\varepsilon \stackrel{iid}{\sim} N(0,1)$$
$$\mu_i \sim N(0,\sigma_{\mu}^2)$$

We set parameters $\beta_0 = 0$, $\beta_1 = 1.65$, $\beta_2 = 1.35$, $\beta_3 = 0.7$, $\beta_4 = -.0.12$ with $\sigma_{\mu} = 1,2,3,4,5$

The simulation study aimed to evaluate the impact of measurement error on the independent variables (regressors) in a regression analysis.

By introducing controlled measurement errors into the regressors x_1 , x_2 , x_3 , and x_4 the simulation study assessed how these errors influenced the accuracy and coverage of the regression model's estimates.

Figure 1: Linear and Non-Linear Mixed effects model with measurement Error



Figure 1 shows the analysis of the investigation between the application of linear and non-linear mixed effects models in scenarios with measurement error. The results are presented visually, showcasing the true data alongside the observed data with fitted models.

In a linear mixed effects model, the relationship between a response variable and a predictor variable is modeled. However, there are random effects that influence the response variable. These random effects are not directly measured, but they can be taken into account by the model. Measurement error can also occur when the predictor variable is not measured perfectly. This can lead to biased estimates of the relationship between the predictor variable and the response variable.

Non-linear mixed effects models are similar to linear mixed effects models, but they allow for the relationship between the response variable and the predictor variable to be non-linear. Measurement error can also occur in non-linear mixed effects models, and it can have similar effects to those in linear mixed effects models.

Overall, the figure suggests that linear and non-linear mixed effects models can be used to account for measurement error. This can help to improve the accuracy of the estimates of the relationship between a response variable and a predictor variable.

4.1 Process Model (Likelihood)

The relationship between the outcome Y and our predictors, including the true variable X_{true} and some non-linear function of Z is given by:

$$Y = \beta_{X_{Obs}} + f(Z) + \eta$$

Where f(Z) is a semi-parametric function of Z and $\eta \sim N(0, \tau^2)$

In the context of Hierarchical models

$Y \mid \beta, f(Z), X_{1i}, X_{2i}$	Model 1
$Y \mid \beta, f(Z), X_{1i}^*, X_{2i}$	Model 2
$Y \mid \beta, f(Z), X_{1i}, X_{2i}^*$	Model 3
$Y \beta, f(Z), X_{1i}^*, X_{2i}^*$	Model 4

Models and Coefficients mean for the parameters

MIXED EFFECTS AND SEMI-PARAMETRIC BAYESIAN INTEGRATION MODELS	MIXED I	EFFECTS AND	SEMI-PARAMETRIC	BAYESIAN INTEGR	ATION MODELS
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	Coefficient	Coefficient	Coefficient	Coefficient Mean for	
	Mean for Land	Mean for	Mean for	Fertility	
	size (β_1)	PH	Moisture	(β_4)	
		(β_2)	(β_3)		
Model 1	1.678021926	0.166164303	0.000168374	0.001890047	
Model 2	1.587009748	0.227480184	-7.23E-05	0.002849426	
Model 3	1.026293296	1.580693002	0.000576071	0.021563858	
Model 4	0.464074057	3.125424642	-0.000271011	0.046263336	
R-Squared	0.9227	0.9155	0.3451	0.9226	
Adjusted R-	0.9034	0.8944	0.1814	0.9033	
Squared					
P-Value	0.002301	0.002755	0.2202	0.002305	

Table 1: Models and Coefficients mean for the parameters

The findings reveal interesting differences between four models. Each model explores the relationship between various factors and an outcome we haven't been told about yet. These factors include land size, PH level, moisture content, and fertility. The results are presented as average values across multiple trials.

For instance, in model one, a larger piece of land (by one unit) is on average linked to a 1.678 increase in the target outcome. The coefficient values for each factor tell a similar story across the models.

Two key metrics help us evaluate how well each model explains the data. R-squared, a value closer to one being better, tells us what proportion of the outcome's variation can be explained by the model. Models one and four have the highest R-squared (around 0.92), suggesting they capture most of the outcome's variance.

Adjusted R-squared considers the number of factors included in the model, penalizing models with too many. It follows the same trend as R-squared here.

Finally, the p-value indicates how likely it is that the observed connections between the factors and the outcome happened by chance. All models have a very low p-value (below 0.05), signifying these relationships are statistically significant.

In conclusion, based on how well they explain the data, models one and four appear strongest. Model two might be less favorable due to a lower R-squared value. Choosing the best model depends on the specific question being asked and the context of the research.

Measurement Error Variability



Figure 2: Estimate of β 's with by measurement error variability

The figure 2 shows the results of a simulation investigating the effect of measurement error variability on the estimation of β . The left side of the figure shows the estimated values of β plotted against the true value, with different colors representing different levels of measurement error variability. The right side of the figure shows the bias and standard error of the estimate of β , plotted against the measurement error variability.

The findings of the simulation are that there is a positive correlation between the estimate of β and the increase in error variability. This means that as the measurement error variability increases, the estimate of β also increases. The increase in error variability is also associated with an increase in the standard error of the estimate of β . This means that the estimates become more spread out as the measurement error variability increases.

It is important to note that this is just a simulation, and the results may not apply to all real-world situations. However, the findings do suggest that measurement error variability can be an important factor to consider when estimating β .

4.2 Bayesian Integration Using Bayes Theorem

In Bayesian Integration, we can postulate the hierarchical models as follows:

$$P(\beta_i, f(Z) | X_{Obs}, Y) \propto P(Y | \beta_i, f(Z), X_{Obs}) \times P(\beta_i, f(Z) | X_{Obs})$$

Therefore,

$$P(\beta_i, f(Z) \mid X_{Obs}, Y) = \int_{\Omega_{\eta}} P(Y \mid \beta_i, f(Z), \eta) \times P(\beta_i, f(Z) \mid \eta) P(\eta \mid X_{Obs}) d_{\eta}$$

We consider a model where outcome *Y* is influenced by *Z* and η follows a semiparametric form based on error-prone predictors *X*.

4.3 Gibbs Sampler

All models were fitted using WinBUGS with the Gibbs Sampler, an MCMC technique for estimating the joint posterior distributions of parameters in the models. The resulting samples approximate the joint posterior distribution and were used for inference about the parameters.



4.3.1 Trace Plot for posterior Inference



parameters

The figure 3 shows the simulation values at each iteration. The chain shows no particular pattern and low autocorrelation. They indicate good mixing and suggest that the sampler is exploring the parameters space effectively





Figure 4: Auto correlation plot for the parameters

In figure 4, the ACF shows a rapid decay and become close to zero for larger lags. This rapid decay of autocorrelation suggests low autocorrelations, good mixing, meaning the chain is exploring the parameter space well, and the samples are approximately independent.

4.4 Model selection

Table 2: Four models with parameters showing land size with other covariates for measurement error variability in optimizing fertilizer application

Parameters	Model 1	Model 2	Model3	Model4
β_1	-1.0245	1.4609	0.1908	-0.2785
β_2	0.1248	0.8675	-0.6782	0.9739
β_3	1.4789	1.2389	-2.6987	1.5738
β_4	-0.8976	-1.3465	1.6729	-0.6826
DIC	2.9683	1.7678	7.8920	2.5038

This table 2 presents the findings of the model comparison for optimizing fertilizer application. Four models were evaluated, considering land size and other covariates to account for measurement error variability.

The Deviance Information Criterion (DIC) was used to compare the goodness-of-fit and model complexity. Lower DIC values indicate a better balance between model fit and parsimony.

Based on the DIC values, Model 2 appears to be the preferred model for fertilizer application optimization (DIC = 1.7678). However, it is crucial to acknowledge that DIC is just one metric for model selection.

4.5 Measurement error variability plot with the selected model

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Figure 5: measurement error variability corrected with the selected model

The figure 5, shows the graph depicts the model's prediction after accounting for some measurement errors. The y-axis appears to show the predicted values, with values increasing from bottom to top. There are multiple data series (representing different groups). The hierarchical natures of the data were well fitted to provide the appropriate fit for the data to achieve the optimal fertilizer application levels in the midst of several covariates.

5. DISCUSSION

This study delved into the impact of measurement error on regression analysis, employing Gaussian process simulations. It investigated linear and non-linear mixed effects models, highlighting their ability to mitigate measurement error's influence on regression estimates.

The findings from model comparisons revealed details in the relationship between various factors and an undisclosed outcome, emphasizing the significance of model selection based on metrics like R-squared, adjusted R-squared, and p-values. Models one and four emerged as strong contenders, whereas model two showed relatively lower explanatory power.

Moreover, the exploration of measurement error variability showcased its correlation with the estimation of β , underlining its importance in model accuracy. Bayesian integration using

hierarchical models and Gibbs sampling facilitated parameter inference, ensuring robustness in the analysis.

The model selection process, guided by the Deviance Information Criterion (DIC), favored Model 2 for optimizing fertilizer application, highlighting its superior balance between goodness-of-fit and model complexity.

Finally, the visualization of measurement error variability corrected with the selected model illustrated the model's predictive capabilities in optimizing fertilizer application amidst diverse covariates. In summary, this study provides insights into the complexities of regression analysis in the presence of measurement error, offering methodological approaches for robust inference and model selection.

6. CONCLUSION

In conclusion, this study conducted a comprehensive exploration of the impact of measurement error on regression analysis, employing Gaussian process simulations. By investigating both linear and non-linear mixed effects models, the research elucidated their effectiveness in mitigating the influence of measurement error on regression estimates with the extension to hierarchical bayesian semi parametric models.

The comparison of models revealed intriguing insights into the relationships between various factors and an undisclosed outcome, emphasizing the importance of thorough model selection guided by metrics such as R-squared, adjusted R-squared, and p-values. Furthermore, the investigation into measurement error variability underscored its correlation with the estimation of β , highlighting its critical role in ensuring the accuracy of regression models. Through Bayesian integration using hierarchical models and Gibbs sampling, the study facilitated robust parameter inference, enhancing the reliability of the analysis.

The model selection process, guided by the Deviance Information Criterion (DIC), identified Model 2 as the preferred choice for optimizing fertilizer application, striking a delicate balance between model fit and complexity. Finally, the visualization of measurement error variability corrected with the selected model offered compelling evidence of the model's predictive capabilities, particularly in optimizing fertilizer application amidst diverse covariates.

In summation, this research contributes valuable insights into the intricacies of regression analysis in the presence of measurement error, offering methodological approaches for robust inference and model selection, with implications for diverse fields reliant on accurate predictive modeling.

DATA AVAILABILITY

Simulation studies were derived and R codes are available on request

AUTHORS' CONTRIBUTION

All authors have contributed significantly to the conception, design and interpretation of the findings presented in this paper. Each author has reviewed and approved the final version of the manuscript.

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CONFLICT OF INTERESTS

The authors declare that there is no conflict of interests.

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