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Stochastic Residual Selection in Simulated Annealing for Clusterwise Panel Optimization

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Abstract

Modeling heterogeneity in panel data requires solving a complex combinatorial partition problem under structural constraints. Although clusterwise regression captures latent group structures with distinct parameters, determining the optimal partition remains computationally challenging due to the vast solution space and susceptibility to local minima. This study proposes a modified simulated annealing (SA) algorithm incorporating a Stochastic Residual Selection (SRS) mechanism, in which candidate units are selected from a high-residual subset rather than deterministically relocating only the unit with the largest residual. The stochastic candidate-size parameter was evaluated using $m = 1$ *and* $m = 5$*, where* $m = 1$ *represents deterministic selection of the largest residual unit, while* $m = 5$ *randomly selects one unit from the five largest-residual units for clusterreassignment. The stochastic perturbation enhances global exploration and improves convergence stability in non-convex optimization landscape. Simulation experiments involving 200 individuals observed over three time periods demonstrate that the proposed SRS-SA outperforms standard SA, achieving an Adjusted Rand Index of approximately 0.95 at 1,000 iterations while producing lower Mean Absolute Bias and Mean Squared Error. An empirical application to improved sanitation data across districts and municipalities in Java, Indonesia, further confirms its effectiveness in identifying latent structural heterogeneity. These findings highlight the robustness and computational efficiency gained through stochastic diversification in metaheuristic optimization for constrained clusterwise panel modeling.*

Keywords: clusterwise regression; metaheuristic optimization; simulated annealing; stochastic optimization; unobserved heterogeneity

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1. Introduction

Panel data analysis is widely used in empirical research because it allows researchers to observe multiple cross-sectional units over time and to capture both between-unit and within-unit variations [1], [2]. One of the central challenges in panel modeling is the presence of unobserved heterogeneity among units, particularly when different individuals, regions, or institutions respond differently to the same explanatory variables [3], [4]. Conventional pooled regression assumes that all units share a common regression structure, whereas fixed effects models allow unit-specific intercepts but still impose homogeneous slope coefficients across units [5], [6]. This assumption may be restrictive in empirical settings where the marginal effects of predictors differ across unobserved subgroups [7], [8].

A more flexible approach is provided by panel models with latent group structures and clusterwise regression. These models assume that cross-sectional units can be classified into a finite number of unobserved groups, where units within the same group share similar regression parameters while parameter heterogeneity is allowed across groups [8-11]. This framework offers a compromise between overly restrictive homogeneous panel models and fully unit-specific regressions, which may suffer from excessive parameterization and limited interpretability [10], [11]. In this sense, clusterwise panel regression is useful for identifying structural heterogeneity while preserving model parsimony and substantive interpretability.

Despite its methodological relevance, clusterwise panel regression involves a complex combinatorial optimization problem. The model requires

simultaneous determination of unit cluster membership and estimation of cluster-specific regression coefficients [12], [13]. In panel data, this problem is further constrained because cluster membership must be assigned at the unit level rather than at the observation level; all time observations belonging to the same unit must remain in the same cluster to preserve longitudinal consistency [8], [14]. As the number of units and clusters increases, the number of possible partitions grows rapidly, making exhaustive search infeasible and increasing the risk of convergence to local optima [15], [16].

Several approaches have been proposed to deal with latent heterogeneity in panel data, including penalized estimation, finite mixture models, and clustering-based procedures [9], [17]. However, many of these approaches may be sensitive to initial values, distributional assumptions, or the complexity of the search space [18], [19]. In clusterwise regression, iterative relocation procedures and greedy search mechanisms can improve local fit but may fail to explore the solution space sufficiently when the objective function is non-convex [12], [20]. Therefore, a robust optimization strategy is required to balance local improvement and global exploration.

Metaheuristic optimization methods provide a practical alternative for solving complex partitioning problems in which conventional deterministic optimization becomes difficult [21], [22]. Simulated annealing (SA) is particularly suitable because it allows occasional acceptance of inferior solutions during the search process, enabling the algorithm to escape local optima [23], [24]. In the context of clusterwise panel regression, SA can be used to explore alternative unit-to-cluster assignments while repeatedly updating cluster-specific regression estimates. However, the effectiveness of SA depends not only on the acceptance probability but also on how candidate moves are generated during the optimization process [25].

In standard residual-based implementations, candidate moves are often generated by selecting the unit with the largest residual and relocating it to another cluster. Although this deterministic largest-residual rule may accelerate short-term reduction of the objective function, it can reduce search diversity and increase the possibility of premature convergence. The algorithm may repeatedly focus on the same poorly fitted unit, leading to oscillation around suboptimal partitions. This limitation is more critical in panel data because moving one unit implies moving all of its time observations simultaneously, so an ineffective move may have a larger impact on the overall partition structure.

To address this computational gap, this study proposes a modified simulated annealing algorithm incorporating a Stochastic Residual Selection mechanism, referred to as SRS-SA. Instead of deterministically selecting only the unit with the largest residual, the proposed method constructs a candidate list consisting of the m units with the largest residuals and randomly selects one unit from this list for reassignment. The candidate-size parameter m controls the degree of stochasticity in the search process. When $m = 1$, the method corresponds to deterministic largest-residual selection, whereas $m > 1$ introduces controlled randomness while retaining residual-based guidance. This mechanism is expected to improve exploration of the partition space without turning the relocation process into a purely random search.

The contribution of this study is threefold. First, it formulates clusterwise panel regression as a constrained partition optimization problem in which cluster membership is consistently assigned at the unit level. Second, it introduces the SRS mechanism into simulated annealing to balance exploitation of high-residual information and stochastic exploration of alternative partitions. Third, it evaluates the proposed method through simulation experiments involving $N = 200$ individuals observed over $T = 3$ periods and through an empirical application to improved sanitation data across districts and municipalities in Java, Indonesia. The performance of the proposed SRS-SA algorithm is compared with standard SA using clustering accuracy, bias, and mean squared error to assess whether the stochastic candidate-selection mechanism improves convergence stability and parameter estimation reliability.

2. Methods

The overall procedure of the proposed SRS–SA framework for clusterwise panel regression is summarized in the flowchart presented in Figure 1. The diagram illustrates the sequential stages of the method, including data input, initialization, the SRS–SA optimization loop, convergence assessment, and final model evaluation. A detailed explanation of each component and computational step in the flowchart is provided in the subsections of this Methods section.

2.1 Mathematical Framework and Objective Function

The fundamental goal of clusterwise panel regression is to partition a set of N cross-sectional units into K latent clusters such that the total sum of squared residuals is minimized. Let y_{it} be the dependent variable and x_{it} be a $p \times 1$ vector of predictors for unit i $(i = 1, \dots, N)$ at time t $(t = 1, \dots, T)$. We assume that each unit i belongs to exactly one cluster C_k for all t. The model for unit i in cluster C_k is expressed in Equation 1.

$$y_{it} = x_{it}'\beta_k + \epsilon_{it} \quad (1)$$

β_k is the vector of regression coefficients specific to cluster k. The optimization problem is defined as finding the partition $\mathbb{C} = \{C_1, C_2, \dots, C_K\}$ that minimizes the global objective function as given in Equation 2.

$$\mathrm{SSE}(\mathbb{C}, \beta) = \sum_{k=1}^{K} \sum_{i \in C_k} \sum_{t=1}^{T} (y_{it} - x_{it}'\beta_k)^2 \quad (2)$$

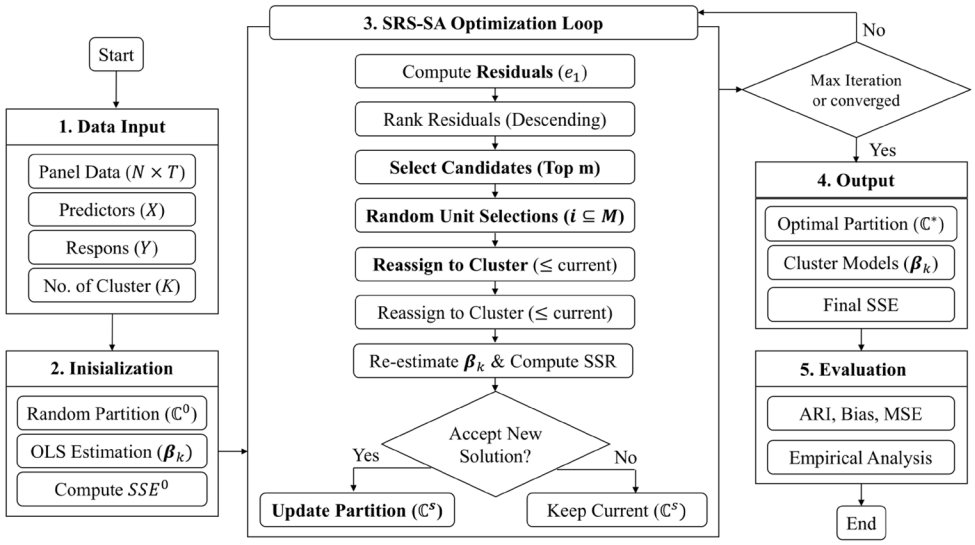


Figure 1 Research framework SRS-SA for clusterwise regression

2.2 Standard Simulated Annealing (SA) Approach

Simulated Annealing is a metaheuristic inspired by the thermodynamic process of cooling solids [18]. In the context of clusterwise regression, the algorithm navigates the combinatorial space of possible partitions by proposing moves transferring a unit from one cluster to another.

In a standard SA implementation, the perturbation step often follows a greedy or semi-deterministic heuristic to accelerate convergence. Specifically, the algorithm identifies the unit i^* that exhibits the highest squared residual as given in Equation 3.

$$e_i^2 = \sum_{t=1}^{T}\left(y_{it} - x_{it}'\hat{\beta}_k\right)^2 \quad (3)$$

This worst-fit unit is then moved to a different cluster. While this efficiently reduces error in the short term, it frequently leads to deterministic oscillations, where the algorithm repeatedly moves the same high-residual unit back and forth between two sub-optimal clusters, effectively becoming trapped in a local minimum.

2.3. Proposed Innovation: Stochastic Residual Selection Simulated Annealing (SRS-SA)

To overcome the limitations of the greedy approach, this study introduces the Stochastic Residual Selection (SRS) mechanism within the simulated annealing framework. Instead of a deterministic choice, we inject a controlled layer of randomness into the selection of candidates for cluster reassignment.

The refined SRS-SA procedure consists of four main steps. At each iteration, the total residual e_i^2 is first calculated for every unit $i = 1, \ldots, N$ and the units are ranked according to their residual values. A candidate list M is then constructed by selecting the top m units with the largest residuals, representing the observations that are most likely to benefit from reassignment. Next, one unit, denoted by i_{rand} is randomly selected from the candidate list to undergo a cluster reassignment, thereby generating a new trial partition $\mathbb{C}_{new}$. Finally, the proposed partition is evaluated using the Metropolis acceptance criterion. The new partition is accepted unconditionally if $\Delta SSE < 0$ indicating an improvement in the objective function. Otherwise, when $\Delta\, SSE \geq 0$ the partition is accepted with probability $P = e^{-\Delta SSE/T_s}$ allowing the algorithm to occasionally accept inferior solutions and thereby reducing the likelihood of becoming trapped in local optima

2.4 Provisions of Writing Equations

The integration of the SRS mechanism provides three critical advantages for panel data modeling. First, it would avoid deterministic cycles. By not focusing exclusively on the maximum residual, the algorithm avoids the effect where a single outlier dominates the search path. This allows the algorithm to reorganize other problematic units that contribute to the global error but are not the absolute worst-fit.

The second advantage is that the SRS might enhance the exploration of the solution space. The stochastic selection acts as a secondary exploration mechanism. While the Metropolis criterion (acceptance probability) allows for worse moves in the energy landscape, the SRS ensures that the starting point of each move is not overly restricted, providing a more robust traversal of the rugged objective function surface. The other significant advantage is its robustness to structural outliers. In panel data, specific units may possess unique trajectories that do not fit any cluster well. A greedy algorithm would exhaust its computational budget attempting to fit these outliers. SRS-SA, conversely, allows the algorithm to occasionally ignore these outliers and focus on optimizing the broader cluster structures.

This approach shares philosophical roots with the candidate list M found in the Greedy Randomized Adaptive Search Procedure (GRASP) and the

diversification strategies in Variable Neighborhood Search (VNS). However, its application specifically to the longitudinal structure of panel data represents a novel contribution to the field of computational statistics.

2.5 Algorithmic Implementation

The proposed algorithm takes as input a panel dataset consisting of the dependent variable Y and independent variables X, the predetermined number of clusters K, the maximum number of iterations MaxIter, and the candidate list size m. The algorithm begins with an initialization step by randomly generating an initial partition $\mathbb{C} = \{C_1, C_2, \dots, C_K\}$. For each cluster, the regression coefficients $\hat{\beta}_{\boldsymbol{k}}$ are estimated using the ordinary least squares (OLS) method. The initial objective value is then computed as $SSE_{old} = SSE(\mathbb{C}^0, \hat{\beta})$, the iteration counter is initialized to $s = 1$, and the initial solution is recorded as the current best solution.

The optimization procedure is subsequently performed iteratively until the maximum number of iterations is reached. In each iteration, the unit-specific residual is first calculated for every cross-sectional unit as $e_i^2 = \sum_{t=1}^{T}\left(y_{it} - x_{it}'\hat{\beta}_k\right)^2$. These residuals are ranked in descending order, and the top m units with the largest residuals are selected to form the candidate list M. One unit i^* is then randomly selected from M and reassigned to a different cluster $k' \neq k$ to generate a trial partition $\mathbb{C}_{\text{new}}$. The regression coefficients of the affected clusters are subsequently re-estimated using OLS, after which the new objective value SSE_{new} is computed. The change in the objective function is evaluated as $\Delta SSE = SSE_{new} - SSE_{old}$.

The trial solution is accepted according to the Metropolis acceptance criterion. If $\Delta SSE < 0$, the new partition improves the objective function and is accepted directly by updating the current partition and objective value $\mathbb{C} = \mathbb{C}_{\text{new}}$ and $SSE_{old} = SSE_{new}$. Otherwise, a random number $u \sim$ U(0,1) is generated, and the trial solution is accepted with probability (\exp(-\Delta SSE/T_s)). Specifically, if $u < e^{-\frac{\Delta SSE}{T_s}}$, the new partition is accepted despite yielding a larger objective value; otherwise, the current partition is retained. This probabilistic acceptance mechanism enables the algorithm to escape local optima by occasionally accepting inferior solutions. After each iteration, the iteration counter is incremented by one.

The algorithm terminates when the number of iterations reaches MaxIter. The final output consists of the optimal cluster partition C together with the corresponding regression coefficients estimated for each cluster.

The candidate-size parameter m controls the balance between exploitation and exploration during the search process. Small values of m focus the search on the units with the largest residuals, whereas larger values increase stochastic exploration by allowing candidate selection from a broader set of poorly fitted units. Therefore, m should be sufficiently small to preserve residual-based guidance while sufficiently large to avoid premature convergence. In this study, $m = 5$ was selected because preliminary simulation results showed higher clustering accuracy and lower estimation error than the deterministic case ($m = 1$).

Some notes could be given concerning some parameters of the algorithm. Choosing $m = 1$, the algorithm converges back to the standard greedy SA, focusing only on the single worst-performing unit. On the other hand, if $m = N$, then the algorithm becomes a purely random SA, where any unit can be chosen for relocation regardless of its fit. This increases exploration but significantly slows down convergence.

3. Results and Discussions

3.1 Simulation Study

To evaluate the performance and robustness of the proposed Stochastic Residual Selection Simulated Annealing (SRS-SA) algorithm, we conduct a controlled simulation study. The objective is to compare the SRS-SA against the standard Simulated Annealing (SA) framework in recovering latent cluster structures and providing unbiased parameter estimates.

We generate a synthetic panel dataset with N = 200 individuals over T = 3 time periods so that the total number of observations is as many as 600 observations. The individuals were partitioned into K=2 clusters with approximately equal numbers of units in each cluster. The data-generating models were specified as follows: Cluster 1 was generated according to $y_{it} = 20 + 0.4x_{1,it} + 0.1x_{2,it} + \epsilon_{it}$, while Cluster 2 followed $y_{it} = 2 + 0.2x_{1,it} + 0.7x_{2,it} + \epsilon_{it}$. Predictors x_k are drawn from a standard normal distribution, and the error term $\epsilon \sim N(0, 0.2)$. We perform 100 simulation replicates, each running for 10,000 iterations.

The performance of the algorithms is assessed using four metrics that capture different dimensions of model quality: clustering accuracy, information efficiency, and parameter reliability. Clustering accuracy was assessed using the Adjusted Rand Index (ARI), which is widely regarded as the standard measure for validating clustering results when the true cluster memberships are known [19]. While the standard Rand Index measures the proportion of agreement between two partitions [20], the ARI adjusts for the probability of grouping units correctly by pure chance. Let n_{ij} be the number of objects in cluster i of the true partition and cluster j of the algorithm's partition. The ARI according to [21] is defined in Equation 4.

$$ARI = \frac{\Sigma_{ij}\binom{n_{ij}}{2} - \frac{\left[\Sigma_i\binom{a_i}{2}\Sigma_j\binom{b_j}{2}\right]}{\binom{n}{2}}}{\frac{1}{2}\left[\Sigma_i\binom{a_i}{2} + \Sigma_j\binom{b_j}{2}\right] - \frac{\left[\Sigma_i\binom{a_i}{2}\Sigma_j\binom{b_j}{2}\right]}{\binom{n}{2}}} \quad (4)$$

a_i is the total number of objects that belong to true cluster i and b_j is the total number of objects that the assigned by the algorithm to cluster j. High accuracy in SSE reduction does not always guarantee that the individual units were assigned to their correct latent groups. The ARI allows us to see if the SRS-SA is structurally superior in identifying the underlying population segments.

Model quality was further evaluated using the Akaike Information Criterion (AIC), which measures the trade-off between model goodness-of-fit and complexity [22]. For clusterwise regression, the AIC penalizes the likelihood based on the number of parameters estimated across all clusters, as defined in Equation 5.

$$AIC = 2[K(p+1)] + (N \times T)\ln\left(\frac{SSE}{N \times T}\right) \quad (5)$$

K is the number of clusters and p is the number of predictors. The AIC helps determine if the algorithm finds a model that is statistically efficient. Since both algorithms use the same K, the AIC will primarily reflect which algorithm reached a lower global minimum of the SSE.

The reliability of parameter estimation was evaluated using the Absolute Bias. Absolute Bias quantifies the systematic deviation of the estimated coefficients from their true values over (R) simulation replicates and is defined in Equation (6) [23] is defined in Equation 6.

$$Absolute\ Bias\ (\hat{\beta}) = \frac{1}{R}\sum_{r=1}^{R}\left|\hat{\beta}_r - \beta_{true}\right| \quad (6)$$

In panel data, if a unit is assigned to the wrong cluster, the resulting $\hat{\beta}$ for that cluster will be far from the true values. Low bias indicates that the SRS-SA successfully isolated the groups, allowing for pure parameter estimation.

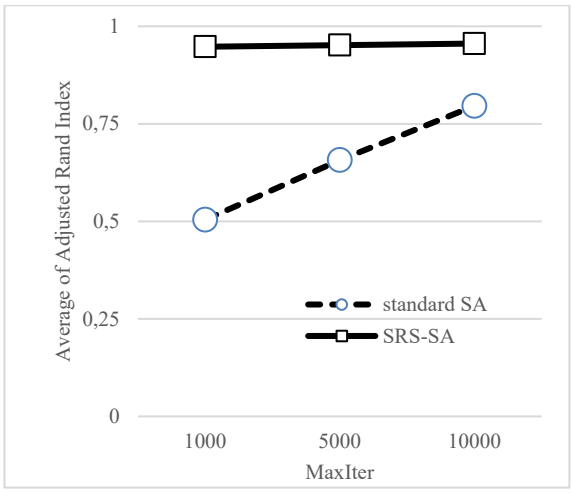
To complement this measure, the Mean Squared Error (MSE) is used to evaluate the overall quality of the parameter estimates by jointly accounting for both estimation bias and variability [24], as defined in Equation 7.

$$MSE\ (\hat{\beta}) = \frac{1}{R}\sum_{r=1}^{R}\left(\hat{\beta}_r - \beta_{true}\right)^2 \quad (7)$$

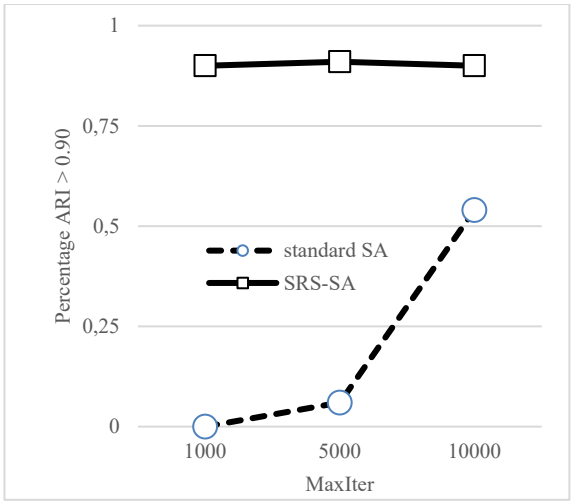
While bias measures how far we are from the truth on average [25], MSE measures how much our estimates scatter [26]. A lower MSE in SRS-SA would prove that the stochastic innovation leads to more stable and reliable results across different data realizations compared to the standard greedy search.

The core of our evaluation lies in the ability of the algorithms to correctly partition the 200 individuals into their respective latent clusters. Figure 2 summarizes the performance of the standard Simulated Annealing (SA) and our proposed Stochastic Residual Selection (SRS-SA) over 100 simulation runs.

Based on the simulation results provided in the figures, the proposed Stochastic Residual Selection Simulated Annealing (SRS-SA) demonstrates a significant leap in both optimization efficiency and robustness compared to the standard Simulated Annealing (SA) framework. The empirical evidence suggests that incorporating a stochastic layer in the selection of high-residual units allows the algorithm to identify the true latent cluster structure with remarkably fewer iterations and higher consistency.



(a)



(b)

Figure 2. Performance comparison between Standard SA and SRS-SA across different iteration thresholds. (a) Average Adjusted Rand Index (ARI) based on 100 simulation replicates, (b) Robustness analysis representing the percentage of replicates achieving high-fidelity clustering (ARI > 0.90)

The first point of interest is the trajectory of the Average Adjusted Rand Index (ARI) across different iteration thresholds (MaxIter). As shown in the results, the SRS-SA algorithm achieves a near-perfect average ARI (approximately 0.95) at just 1000 iterations and maintains this high level of precision as the computational budget increases. In sharp contrast, the standard SA begins with a substantially lower average ARI of approximately 0.50 at 1000 iterations and exhibits a slow, linear improvement, reaching only about 0.80 even after 10000 iterations. This indicates that the SRS-SA is not only more accurate but also computationally efficient, reaching a superior solution

in a fraction of the time required by the conventional approach.

Furthermore, the robustness of the SRS-SA is clearly evidenced by the percentage of replicates achieving an ARI greater than 0.90. This metric represents the success rate of the algorithm in finding the near-global optimum. The SRS-SA maintains a consistent success rate of approximately 90% across all tested iteration levels. Conversely, the standard SA fails completely to reach the 0.90 ARI threshold at 1000 and 5000 iterations, only managing to succeed in roughly 55% of the trials when the iterations are increased to 10000. This difference highlights that the standard SA is highly sensitive to initial partitions and frequently becomes trapped in local optima, whereas the SRS-SA's stochastic selection mechanism consistently navigates toward the correct group structure.

The sensitivity of the proposed algorithm to the candidate-size parameter was evaluated by comparing $m = 1$ and $m = 5$. The results indicate that $m = 5$ consistently achieves higher ARI values and lower estimation errors than $m = 1$, suggesting that moderate stochasticity improves the algorithm's ability to escape local optima while preserving residual-based guidance. From a computational perspective, the impact of m on execution time is relatively limited because residuals must still be calculated for all units at every iteration. Consequently, computational cost is driven primarily by the number of observations and the maximum number of iterations rather than by the candidate-size parameter itself.

Table 1. Independent Sample t-Test Results for ARI Values at Different Iteration Levels

Number of iteration	T value	P-value	
1000	-33.61	<0.00	***
5000	-14.78	<0.00	***
10000	-6.71	<0.00	***

Significant codes: *p<0.05, **p<0.01, ***p<0.001

To further assess whether the observed performance differences are statistically significant, independent sample t-tests were conducted to compare the ARI values produced by the two algorithms at each iteration level (Table 1). The results reveal highly significant differences in favor of the proposed method across all experimental settings. At 1000 iterations, the test statistic reached $t = -33.61$ ($p < 0.00$), indicating an extremely large performance gap between SRS-SA and the standard SA. Similar findings were obtained at 5000 iterations ($t = -14.78, p < 0.00$) and 10000 iterations ($t = -6.71, p < 0.00$). These results provide strong statistical evidence that the superior performance of SRS-SA is not attributable to random variation but reflects a genuine improvement in clustering accuracy.

Although the magnitude of the t-statistic decreases as the number of iterations increases, all comparisons remain highly significant. This pattern is consistent with the convergence behavior observed in the simulation study. As the standard SA is allowed more iterations, its ARI gradually improves and approaches that of SRS-SA, thereby reducing the performance gap between the two methods. Nevertheless, the persistence of significant differences even at 10000 iterations demonstrates that the stochastic residual selection mechanism continues to provide a meaningful advantage in recovering the true cluster structure.

Overall, the combination of higher average ARI values, substantially greater success rates in achieving near-perfect clustering solutions, and consistently significant t-test results confirms that the SRS-SA algorithm offers a more effective and reliable optimization strategy for clusterwise linear regression. By introducing stochasticity into the residual-based neighborhood generation process, the proposed method enhances exploration of the solution space while preserving the strengths of residual-guided search, resulting in faster convergence, improved cluster recovery, and greater robustness against local optima.

The thematic consistency of these results confirms the theoretical rationale behind the stochastic innovation. In the standard SA, the deterministic focus on the maximum residual likely causes the search to oscillate around sub-optimal partitions between problematic units. By selecting from a pool of high-residual candidates rather than just the single worst-fit unit, the SRS-SA provides the necessary shaking effect to the objective function's energy landscape. This allows the algorithm to reorganize the cluster memberships more holistically, ensuring that the longitudinal patterns of the 200 individuals are correctly identified regardless of the starting configuration or the limited number of iterations.

Table 2. Comparison of Mean Absolute Bias and MSE

Coefficient	Mean Absolute Bias		Mean Square Error	
	Standard SA	SRS-SA	Standard SA	SRS-SA
$\beta_{0,1}$	3.03	0.56	22.46	2.75
$\beta_{0,2}$	2.68	0.66	17.47	3.72
$\beta_{1,1}$	0.91	0.31	2.55	0.98
$\beta_{1,2}$	0.97	0.29	2.80	0.93
$\beta_{2,1}$	0.91	0.30	2.54	0.99
$\beta_{2,2}$	0.99	0.29	2.82	0.88

Beyond clustering accuracy, the performance of the algorithms is further scrutinized through their ability to provide precise and unbiased parameter estimates. The results for Mean Absolute Bias and Mean Square Error (MSE) for the panel regression coefficients are presented in Table 2. A comparative analysis reveals a substantial gap between the two algorithms, particularly regarding the intercept terms β_0. For the first cluster ($\beta_{0,1}$), the proposed SRS-SA algorithm achieves a significantly lower Mean Absolute Bias of 0.56 compared to the 3.03 observed in the standard SA. This trend is mirrored in the MSE values, where the SRS-SA records a precision of 2.75, while the standard SA exhibits a high error of 22.46. Similarly, for the second cluster intercept $\beta_{0,2}$, the SRS-SA maintains superior accuracy with a bias of 0.66 and an MSE of 3.72,

whereas the standard SA results in a bias of 2.68 and an MSE of 17.47. The estimation of slope coefficients (β_1 and β_2) across both clusters further demonstrates the robustness of the stochastic innovation.

These findings are intrinsically linked to the Adjusted Rand Index (ARI) results discussed previously. The higher misclassification rate of the standard SA, which failed to reach a high ARI consistently, leads to parameter contamination between clusters. When units are incorrectly assigned, the regression model for one cluster is influenced by data belonging to another, resulting in the high levels of bias and MSE observed in Table 2. Conversely, the high ARI stability of the SRS-SA (near 0.95) ensures that the regression coefficients are estimated from correctly partitioned, homogeneous groups. This confirms that the stochastic selection mechanism is a critical prerequisite for obtaining reliable structural parameters in heterogeneous panel data environments.

Table 3. Independent Sample t-Test Results Comparing the Estimation Accuracy of Standard SA and SRS-SA Based on Absolute Bias and MSE

Metric	Coefficient	T value	p-value	
Absolute bias	$\beta_{0,1}$	20.12	<0.00	***
	$\beta_{0,2}$	20.36	<0.00	***
	$\beta_{1,1}$	1.04	0.30	
	$\beta_{1,2}$	1.72	0.09	
	$\beta_{2,1}$	1.20	0.23	
	$\beta_{2,2}$	1.81	0.07	
MSE	$\beta_{0,1}$	7.22	<0.00	***
	$\beta_{0,2}$	8.69	<0.00	***
	$\beta_{1,1}$	-2.77	0.01	*
	$\beta_{1,2}$	-2.66	0.01	*
	$\beta_{2,1}$	-2.76	0.01	*
	$\beta_{2,2}$	-2.67	0.01	*

Significant codes: *p<0.05, **p<0.01, ***p<0.001

To further evaluate whether the observed differences in estimation performance are statistically significant, independent sample t-tests were conducted for both Absolute Bias and MSE across all regression coefficients. The results, presented in Table 3, indicate statistically significant differences between SRS-SA and the standard SA for the intercept parameters under the Absolute Bias criterion, while several slope coefficients did not exhibit significant differences. This finding suggests that the proposed SRS-SA method provides more accurate estimation of cluster-specific intercepts, whereas improvements in slope estimation are less pronounced. One possible explanation is that the true slope coefficients across clusters are relatively similar, making the underlying cluster structures inherently more difficult to distinguish based solely on covariate effects. Consequently, improvements in cluster recovery may not always translate into sufficiently large reductions in bias for certain slope parameters.

In contrast, the MSE results reported in Table 3 show statistically significant differences for most regression coefficients, indicating greater estimation precision under SRS-SA. These findings suggest that even when the average bias of some slope estimates is not substantially different between the two algorithms, the proposed method consistently produces more stable parameter estimates with lower variability. Therefore, the stochastic residual selection mechanism contributes not only to improved cluster recovery but also to enhanced estimation precision. Taken together, the t-test results provide additional statistical evidence that the superior clustering performance of SRS-SA leads to more reliable estimation of the underlying panel regression coefficients.

The simulation study provides compelling evidence for the efficacy of the Stochastic Residual Selection Simulated Annealing (SRS-SA) algorithm in the context of clusterwise panel regression. Across 100 replicates, the proposed method demonstrates a remarkable balance of speed, accuracy, and robustness. By introducing a stochastic layer into the selection of high-residual units, the algorithm successfully navigates the complex, non-convex energy landscape of panel data partitions, effectively avoiding the local optima that frequently trap the standard SA approach.

The superiority of the SRS-SA is most evident in its convergence properties. While the standard SA requires a large iteration budget and still exhibits high variance in its results, the SRS-SA achieves near-perfect latent structure recovery even at a lower iteration threshold. This stability translates directly into high-fidelity parameter estimates, as evidenced by the significantly lower Bias and MSE values across all regression coefficients. The stochastic innovation effectively provides a shaking mechanism that allows the algorithm to reorganize clusters holistically rather than being fixated on individual extreme outliers.

Ultimately, this research highlights that addressing unobserved heterogeneity in panel data requires more than just model flexibility; it requires robust optimization heuristics. The SRS-SA offers a powerful tool for researchers to identify distinct subgroup dynamics accurately. By ensuring that clustering and regression estimation are performed with high global precision, this method provides a more trustworthy foundation for strategic planning and policy interventions where different cross-sectional units respond differently to predictor variables.

Building on these methodological contributions, the following section presents the empirical implementation of the proposed framework. A crucial first step in this implementation is the determination of the optimal number of clusters, as the effectiveness of clusterwise panel regression critically depends on the ability to appropriately balance heterogeneity representation and model parsimony.

3.2 Empirical Implementation

Determining the optimal number of clusters constitutes a fundamental step in clusterwise panel regression, as it directly affects the model's ability to capture structural heterogeneity across regions while preserving

parsimony. Selecting too few clusters results in excessive pooling, whereby distinct regional mechanisms are forced into a homogeneous framework, leading to biased and overly averaged estimates [27]. Conversely, selecting too many clusters risks over-partitioning, increasing model complexity, reducing interpretability, and potentially inducing overfitting [28]. To balance these competing concerns, this study determines the optimal number of clusters by jointly considering goodness-of-fit measures and information criteria, namely the adjusted R-squared (adj-R^2), Akaike Information Criterion (AIC), corrected AIC (AICc), and Bayesian Information Criterion (BIC).

The empirical results reveal a monotonic increase in adj-R^2 as the number of clusters increases from $K = 2$ to $K = 10$. Specifically, adj-R^2 rises from 0.50 at $K = 2$ to 0.93 at $K = 10$, indicating a substantial improvement in explanatory power as cross-sectional heterogeneity is progressively accommodated. This pattern suggests that the relationship between sanitation access and socio-economic determinants in Indonesia is fundamentally heterogeneous and cannot be adequately represented by a single global regression model. However, when the number of clusters is increased further to $K = 11$, adj-R^2 exhibits a slight decline. Although numerically small, this decrease is conceptually important, as adj-R^2 explicitly penalizes model complexity. The observed decline therefore indicates that the additional cluster fails to provide sufficient explanatory gains to justify the increase in model parameters.

This conclusion is strongly reinforced by the behavior of the information criteria. All three measures AIC, AICc, and BIC reach their global minimum at $K = 10$ and increase when the number of clusters is expanded to $K = 11$. Notably, the increase in BIC is particularly pronounced, reflecting its stronger penalty for model complexity. Given that BIC is widely employed to guard against overfitting in latent structure models, this pattern provides compelling evidence that additional clustering beyond $K = 10$ leads to over-segmentation rather than the identification of substantively distinct structural regimes. Taken together, these results identify $K = 10$ as the optimal balance between model fit and parsimony, consistent with the theoretical objective of clusterwise regression to uncover a finite number of meaningful latent regimes.

Based on the evidence presented in Table 4, the estimation results indicate that the fixed effects clusterwise panel regression with ten clusters provides the most appropriate specification for explaining variations in access to improved sanitation (Y) across districts and municipalities. The signs of the estimated coefficients describe the direction of influence, whereby negative coefficients indicate that increases in the corressponding variables reduce sanitation coverage, while positive coefficients reflect enhancing effects. Statistical significance levels (***, **, *, .) denote the reliability of these relationships. Overall, average years of schooling (X_2) and per capita expenditure (X_3) emerge as the most consistently significant determinants across clusters, predominantly exerting positive effects, thereby underscoring the central role of human capital and economic capacity in improving sanitation outcomes. In contrast, the poverty rate (X_1) and the open unemployment rate (X_4) display heterogeneous effects across clusters, with both positive and negative signs observed, reflecting distinct structural mechanisms operating within different regional groups. This heterogeneity directly violates the assumption of slope homogeneity and further justifies the use of a clusterwise modeling approach.

Table 4. Model Selection Criteria for Determining the Optimal Number of Clusters

Cluster	Adj-R^2	AIC	AICc	BIC
2	0.50	805	806	848
3	0.59	739	741	801
4	0.73	603	606	684
5	0.82	455	459	556
6	0.86	383	389	503
7	0.88	328	336	467
8	0.90	256	267	415
9	0.91	227	241	405
10	0.93	163	180	361
11	0.92	174	195	391

From a regional perspective, Cluster 1 is largely composed of urban and peri-urban districts and municipalities with relatively strong educational foundations, where poverty negatively affects sanitation outcomes but can be partially offset by higher educational attainment, highlighting the role of education-driven health awareness and behavioral change. Cluster 2 includes economically active regions in which per capita expenditure significantly supports sanitation improvements, although labor market instability and uneven returns to education constrain their effectiveness. Cluster 3 is dominated by metropolitan areas and large cities, where sanitation outcomes are influenced more by education and urban social dynamics than by poverty, reflecting relatively broad access to public services. In contrast, Cluster 4 represents structurally constrained regions in which both poverty and education exert negative effects on sanitation, rendering sanitation outcomes highly sensitive to economic conditions and the adequacy of public infrastructure.

Cluster 5 represents the most vulnerable sanitation regime, characterized by very large and negative coefficients for poverty and education, indicating that sanitation outcomes in these regions are highly sensitive to socio-economic fluctuations. Cluster 6 is predominantly rural, where education emerges as the primary driver of sanitation improvements, while the effect of poverty remains relatively weak. Cluster 7 exhibits a distinctive pattern in which poverty has a positive association with sanitation outcomes, suggesting the presence of compensatory policies or social programs that help sustain sanitation access despite higher poverty levels. Cluster 8 reflects densely populated and industrialized regions, where labor

market pressures and residential congestion constrain sanitation improvements even amid rising education and economic capacity. Cluster 9 is dominated by large metropolitan areas that are highly sensitive to labor market conditions, whereas Cluster 10 represents regions with relatively strong adaptive capacity, in which education and per capita expenditure consistently promote sanitation improvements despite persistent socio-economic pressures.

Table 5. Coeffisients and Cluster Member

Cluster	B0	B1	B2	B3	B4	Cluster Member
1	-2.88 e+00 ***	-4.08 e-02 **	5.70 e-01 ***	5.51 e-05	-4.59 e-02 *	Bangkalan, Banyumas, Blitar, Cianjur, Gresik, Karawang, Kota Batu, Kota Salatiga, Kota Surabaya, Kota Tegal, Kuningan, Malang, Mojokerto, Pekalongan, Serang, Sukoharjo, Tulungagung
2	7.97 e+00 ***	-2.84 e-02	-4.51 e-01 ***	7.66 e-05 *	-1.37 e-01 ***	Banyuwangi, Kota Bandung, Kota Sukabumi, Magelang, Ngawi, Pangandaran, Pasuruan, Tuban
3	1.09 e+00	-1.22 e-03	3.17 e-01 ***	2.18 e-05	1.00 e-01 ***	Cirebon, Jember, Kota Banjar, Kota Bekasi, Kota Cirebon, Kota Jakarta Selatan, Kota Jakarta Timur, Kota Semarang, Kota Tangerang, Probolinggo, Purbalingga, Subang, Sumenep, Tegal, Temanggung
4	5.44 e+00 ***	-1.92 e-01 ***	-4.07 e-01 ***	1.50 e-04 ***	3.34 e-01 ***	Brebes, Jepara, Kota Jakarta Barat, Kota Tasikmalaya, Situbondo, Sumedang
5	2.42 e+01 ***	-1.05 e+00 ***	-3.74 e+00 ***	1.78 e-03 ***	2.02 e-01 *	Indramayu, Kota Madiun, Kota Tangerang Selatan, Pati, Sidoarjo
6	-4.37 e+00 *	-6.62 e-02	8.17 e-01 ***	1.98 e-04	1.27 e-01 *	Banjarnegara, Batang, Cilacap, Purworejo, Wonosobo
7	7.87 e-01	8.62 e-02 ***	5.27 e-01 ***	-8.54 e-05 *	3.23 e-02	Bojonegoro, Grobogan, Jombang, Kediri, Kota Kediri, Kota Mojokerto, Kota Pasuruan, Kota Pekalongan, Kota Serang, Kota Yogyakarta, Kudus, Kulon Progo, Lumajang, Madiun, Magetan, Ponorogo, Semarang
8	1.56 e+00	3.50 e-02 *	7.44 e-01 ***	-1.15 e-04 ***	-2.53 e-01 ***	Bantul, Bekasi, Blora, Boyolali, Demak, Gunung Kidul, Karanganyar, Kebumen, Klaten, Kota Depok, Lamongan, Pemalang, Purwakarta, Rembang, Sampang, Sragen, Tangerang, Wonogiri
9	-5.10 e-01	7.68 e-02 ***	2.12 e-01 ***	1.66 e-04 ***	-2.12 e-0	Bandung, Bandung Barat, Bogor, Garut, Kepulauan Seribu, Kota Bogor, Kota Cimahi, Kota Jakarta Pusat, Kota Jakarta Utara, Kota Magelang, Kota Malang, Kota Surakarta, Pacitan, Pandeglang, Tasikmalaya
10	-5.39 e+00 ***	1.84 e-01 ***	9.02 e-01 ***	-9.66 e-06	1.52 e-01 ***	Bonodowo, Ciamis, Kendal, Kota Blitar, Kota Cilegon, Kota Probolinggo, Lebak, Majalengka, Nganjuk, Pamekasan, Sleman, Sukabumi, Trenggalek

Significant codes: *p<0.05, **p<0.01, ***p<0.001

Table 5 further demonstrates that the determinants of improved sanitation are not uniform across clusters. Although the same set of explanatory variables is included in each cluster-specific regression model, the variables that are statistically significant, as well as the direction and magnitude of their coefficients, differ across clusters. This indicates that districts and municipalities grouped within different clusters are characterized by distinct socio-economic mechanisms affecting sanitation outcomes. From a policy perspective, these findings suggest that a uniform intervention across regions may not be optimal. Instead, policymakers can use the cluster-specific results to identify the most relevant determinants for each group of regions and prioritize interventions accordingly. For example, clusters in which education is a dominant determinant may require stronger education- and awareness-based interventions, whereas clusters that are more strongly associated with economic capacity, poverty, or labor-market conditions may require different policy priorities. Thus, the clusterwise approach provides an empirical basis for designing more targeted, efficient, and context-specific sanitation policies.

To further contextualize the empirical findings, Figure 3 presents the spatial distribution of the identified clusters across Indonesian districts and municipalities. This visualization complements the cluster-specific regression results by illustrating how regions with similar structural sanitation regimes are geographically distributed, thereby providing an intuitive link between the estimated latent groups and their real-world spatial manifestation.

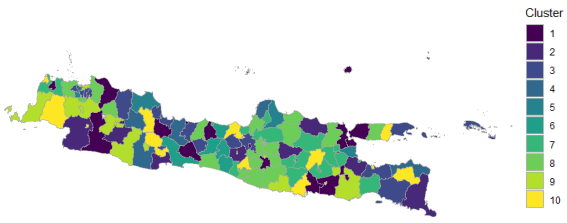


Figure 3. Spatial Distribution of the Ten Sanitation Clusters Across Districts and Municipalities in Java

Notably, the spatial pattern reveals that regions belonging to the same cluster are not necessarily geographically contiguous, reinforcing the notion that sanitation disparities are driven by structural characteristics rather than purely spatial proximity.

This clustering approach is highly relevant, as it demonstrates that the determinants of improved sanitation are not uniform across regions. In the absence of clustering, policies based on a single global model

risk producing misleading average effects and suboptimal interventions. By identifying distinct clusters, policymakers can design more targeted sanitation strategies, such as prioritizing health education in rural areas, strengthening labor market conditions in urban settings, or investing in basic infrastructure in regions with high structural vulnerability. From a societal perspective, this approach contributes directly to improvements in public health, environmental quality, and overall social welfare. Overall, the clustering results provide a strong empirical foundation for more equitable, efficient, and locally responsive sanitation development planning.

4. Conclusions

This study addresses the critical challenge of unobserved slope heterogeneity in panel data by proposing the Stochastic Residual Selection Simulated Annealing (SRS-SA) algorithm for clusterwise regression. While traditional panel models often oversimplify the data through global homogeneity or restrict heterogeneity only to the intercept, our approach allows for the simultaneous discovery of latent groups and their specific structural models. The core innovation introducing a stochastic selection layer for high-residual units effectively mitigates the limitations of standard greedy heuristics, which are prone to deterministic oscillations and local optima.

The simulation results provide robust evidence of the proposed method's superiority. SRS-SA achieved high-fidelity clustering (ARI $>$ 0.90) with remarkable consistency, even at low iteration thresholds where the standard SA failed to converge. This structural accuracy directly translated into more reliable parameter estimates, as evidenced by a substantial reduction in both Absolute Bias and Mean Square Error compared to the conventional approach4. These findings suggest that SRS-SA is a powerful and efficient tool for researchers dealing with complex, heterogeneous longitudinal data. Despite these promising findings, this study has several limitations. The simulation experiments were conducted under a moderate-scale setting with $N = 200$ cross-sectional units and $T = 3$ time periods. Although this setting is sufficient to evaluate the proposed algorithm under controlled conditions, its performance for substantially larger and higher-dimensional panel datasets remains to be further investigated. In addition, the simulation design assumes normally distributed error terms. Therefore, future research should validate the proposed SRS-SA algorithm using larger panel structures and alternative error distributions, including skewed, heavy-tailed, and other non-Gaussian disturbances.

While the simulation results provide robust evidence under controlled experimental conditions, the stated limitations indicate the importance of further assessing the proposed algorithm in applied settings. Accordingly, the empirical analysis provides additional validation for the proposed fixed-effects clusterwise panel regression framework when implemented on real-world panel data.

The empirical results provide strong validation for the proposed fixed-effects clusterwise panel regression framework. The selection of ten clusters, supported consistently by adjusted R-squared and multiple information criteria, confirms that regional sanitation outcomes cannot be adequately explained by a single homogeneous model. Instead, the implementation reveals substantial heterogeneity in both the magnitude and direction of covariate effects across clusters, demonstrating that the proposed SRS–Simulated Annealing approach is effective in uncovering latent structural differences among districts and municipalities.

The cluster-specific estimation results further indicate that education and per capita expenditure emerge as the most robust determinants of improved sanitation across clusters, although their relative importance varies by regional context. In contrast, poverty and unemployment exhibit heterogeneous and sometimes counterintuitive effects, reflecting the presence of distinct socio-economic mechanisms, institutional arrangements, and policy environments across regions. These findings highlight that sanitation outcomes are shaped by complex interactions between economic capacity, human capital, and labor market conditions, which differ markedly across latent regional regimes.

From a methodological perspective, the results underscore the limitations of conventional pooled or homogeneous panel models in the presence of unobserved heterogeneity. The clusterwise approach adopted in this study not only improves model fit but also enhances interpretability by allowing inference to be conducted within structurally coherent regional groups. Substantively, the identification of distinct sanitation clusters provides an empirically grounded basis for differentiated policy design, supporting more targeted, efficient, and context-sensitive interventions aimed at improving sanitation outcomes and reducing regional disparities. From a computational standpoint, the proposed SRS-SA framework further demonstrates improved convergence robustness and solution stability in high dimentional partition optimization problems, reinforcing its contribution to metaheuristic optimization for constrained clustering applications.

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