FZStats v1.0: a raster statistics toolbox for simultaneous management of spatial

stratified heterogeneity and positional dependence in Python

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Abstract: Based on the traditional Focal Statistics and Zonal Statistics tools of mainstream GIS software, we developed a raster statistics toolbox named FZStats v1.0 using Python3 and QT5. The main contributions of this study are as follows. Firstly, the development of a specialized spatial analysis toolset designed to comprehensively address stratified heterogeneity, positional dependence, and their combinations, thereby addressing gaps in existing Focal and Zonal methods that individually tackle stratified heterogeneity and positional dependence problems. Secondly, our toolset features a user-friendly interface and structure, integrates both existing and enhanced spatial statistical methods, supports multi-processing and batch processing capabilities, and provides users with the flexibility to select calculation methods tailored to their computer configurations and application requirements. Thirdly, the newly proposed Focal-Zonal Mixed Statistics method demonstrates superior predictive accuracy compared to the traditional Focal Statistics and Zonal Statistics methods in geothermal detection, which preliminarily showcases the advantages of this new approach. Additionally, we discussed the advantages, robustness, and advancements of the Focal-Zonal Mixed Statistics method, concluding that the development of this new method and toolset is necessary and holds substantial potential for applications across diverse fields. **Abstract:** Focal and Zonal Statistics are fundamental tools in GIS for characterizing spatial patterns, yet they have traditionally addressed spatial stratified heterogeneity (SSH) and spatial positional dependence (SPD) in isolation. To overcome this limitation, we introduce FZStats v1.0, a Python 3/QT5-based toolbox that not only integrates conventional Focal and Zonal statistics, but also implements a novel Focal–Zonal Mixed Statistics approach capable of jointly capturing both SSH and SPD. First, we formally develop the Focal-Zonal Mixed Statistics model to address stratified heterogeneity, spatial dependence, and their interactions within a unified framework—filling a key methodological gap left by traditional approaches that cannot accommodate their co-occurrence in real-world spatial data. Second, FZStats v1.0 provides a user-friendly graphical interface for flexible configuration of neighborhood window shapes (e.g., rectangular, circular, elliptical), sizes, and statistical operations (e.g., mean, percentiles). It also supports multiprocessing and batch operations, enabling scalable computation across diverse spatial analysis tasks. Third, we validate the effectiveness and robustness of the new method through a geothermal anomaly detection case study. Across multiple years, seasons, representative target sizes, and local window radii, the Focal-Zonal Mixed Statistics consistently outperforms both Focal and Zonal Statistics, demonstrating its superior capability in enhancing anomaly signals under complex spatial conditions. In summary, FZStats v1.0 is not only a theoretically grounded and methodologically novel tool, but also a highly adaptable and practical solution for spatial data analysis in diverse application domains. **Keywords:** Spatial Statistics; Raster Operations; Spatial Stratified Heterogeneity; (SSH); Spatial Positional Dependency; (SPD); Focal/Zonal Statistics.

1 Introduction

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The advent of Geographic Information Systems (GIS) marksrepresent a milestone in the evolution of geography-by providing a new paradigm for the integrated management, analysis, and visualization of spatial data (Goodchild, 1992; Bernhardsen, 2002; Longley et al., 2015). As a core function of vital analytical module within GIS-software, spatial statistics provide powerful methods and tools that enable researchers to quantify and decision-makers to analyzeinterpret spatial patterns and associations relationships on the Earth's surface

54 comprehensively and accurately. Spatial heterogeneity and positional dependence are two fundamental characteristics to be considered in spatial data processing (Goodchild and Haining, 55 2004). with unprecedented precision (Fischer & Getis, 2010; Fotheringham & Rogerson, 2013). 56 With continued advances in GIS technology, investigators can now more easily explore the 57 distribution, temporal evolution, and driving mechanisms of spatial variables; and spatial 58 statistical theories and methods play an increasingly prominent role in geographical studies. 59 Two foundational concepts in spatial statistical analysis are spatial heterogeneity and positional 60 dependence (Goodchild & Haining, 2004). Correspondingly, Zonal Statistics and Focal 62 (Neighborhood) Statistics areoffer two essential methods of spatial statistical analysis. The former can be achieved through a model that involves partitioning complementary approaches. 63 Zonal Statistics partitions raster dataunits representing the target variable into several discrete 64 65 zones based on predefined rules or attributes, performing statistical analyses on the raster eells schemes, computes summary metrics such as mean, maximum, minimum, and sum within 66 each zone, and then outputting renders the results as a mosaic raster layer (Singla and Eldawy, 67 2018; Haag et al., 2020; Winsemius and Braaten, 2024). The latter, also known as In contrast, 68 Focal Statistics defines a neighborhood or local window statistics, takes around each raster cell 69 as the center and extends a specified range surrounding the center to form a local window 70 according to the designated specified window shape and size; it performs statistical analyses on 71 the raster cells, calculates the same set of summary metrics within that neighborhood, and 72 assigns the resulting value to the central cell; by sliding this window and then outputs the results 73 as a mosaic raster layer across all locations, it thereby quantifies how these statistics vary with 74 the window's movement (Mathews and & Jensen, 2012; Kassawmar et al., 2019; Zhang et al., 75 2021). The calculated statistics for both zonal and focal methods are similar, including the mean, 76 maximum, minimum, sum, and so on. 77

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Currently, the mainstream Mainstream GIS software platforms including such as ArcGIS

and QGIS provide toolinclude dedicated modules such as for Zonal Statistics and Focal Statistics and Zonal Statistics, both of which have promoted the usage of these two methods been widely adopted in practice. From an application perspective standpoint, Zonal Statistics primarily address deals with spatial stratified heterogeneity (SSH), which can be detected) by dividing partitioning the target variable though study area into zones based on environmental characteristic classified variables characteristics, thereby capturing SSH (Wang et al., 2016; Wang and Xu, 2017; Gao et al., 2022). For instance, the actual vegetation growth or potential growth of vegetation may vary significantly due to different environmental conditions such as often varies markedly among zones delineated by slope and aspect, which are key drivers of vegetation dynamics (Zhang et al., 2018, 2019; Xu et al., 2020). With respect to Conversely, Focal Statistics, it focuses on spatial position positional dependence (SPD), which can be addressed or at least weaken by introducing the local windows or geographic weights) by employing moving-window or geographically weighted techniques to detect and mitigate positional effects (Tobler, 1970; Wolter et al., 2009; Wagner et al., 2018). For example, even soils or rocks with the same texture generally exhibit variations in geochemical element content due to their different spatial locations; however, these differences variations that diminish with decreasing distance, indicating that these attributes are dependent on spatial position reflecting underlying positional dependence; consequently, spatial interpolation of element concentrations typically assigns greater weight to nearer samples (Krige and Magri, 1982; Trangmar et al., 1986; Zuo, 2014). In our real world practice, SSH and SPD may coexist, with the former exhibiting often co-

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In our real worldpractice, SSH and SPD may coexist, with the former exhibiting often cooccur, manifesting as abrupt changes and the latter exhibiting and gradual changes. For example, due to variations in land-sea distribution, solar radiation, and altitude respectively. At broad scales, terrestrial vegetation exhibits strong patterns illustrate SPD through meridional, latitudinal, and vertical zonalaltitudinal gradients driven by land-sea distribution patterns

respectively, solar radiation, and elevation (Qiu et al., 2013; Dong et al., 2019; Eddin and Gall, 2024), which explains the significant SPD in vegetation coverage. Meanwhile, due to the influence of). Conversely, local topography, microclimate, and human activities, the activity introduce sharp boundaries in vegetation coverage differences caused by these factors do not entirely manifest as gradual changes. Typical evidence includes phenomena such as vegetation on-cover, generating SSH—for example, stark contrasts between shady and sunny slopes generally shows SSH (Álvarez-Martínez et al., 2014; Zhang and Zhang, 2022;) and significant differences between urban and rural landscapes (Zhang et al., 2023b). Furthermore, due to differences in formation age, there are significant variations Similarly, in material across strata, which is a major reason for the SSH of mineral resources geology, stratigraphic age differences produce SSH in resource distribution (Zhao Pengda, 2006; Zuo, 2020). Subsequently, under the influence of), while internal and external geological processes, the distribution of impart SPD to mineralization elements often exhibits SPD characteristics patterns (Cheng, 2006, 2012), and Geostatistics and Kriging methods were developed to explain this phenomenon as modeled by geostatistics and kriging (Krige, 1951; Goovaerts, 1997; Müller et al., 2022). Therefore, when dealing with problems involving spatial statistics, it is necessary to considereffective spatial statistical analysis must integrate both SSH and SPD-simultaneously. Some scholars have noted this issue and developed certain improved models in their respective fields to overcome the To address these challenges posed by solely considering SSH or SPD. Professor Zhu and his group expanded upon, previous studies have integrated SSH and SPD, developing specialized hybrid models for specific spatial-statistical objectives. For example, Zhu et al. (2019) extended traditional spatial interpolation methods, which typically focus normally focused solely on spatial dependence, by introducing constraints derived from environmental similarity (Zhu et al., 2019). They further proposed constraints, and formalized the "Third Law of Geography", which states that the more geographically similar

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contexts yield similar the geographic configurations of locations, the more similar the values (processes) of the target-variable at these locations (values (Zhu et al., 2018; Zhu et al., 2020). Meanwhile, ProfessorIn a similar vein, Zhang and his group enhanced traditionalet al. (2019) incorporated spatial sliding-window techniques into vegetation potential assessment-models, which typically only consider similar habitat conditions, by incorporating spatial sliding window techniques (Zhang et al., 2019). This development led to a model for assessing vegetation restoration potential based on local windows, simultaneously considering, resulting in a model that simultaneously considers spatial proximity and environmental similarity (Xu et al., 2020; Zhang, 2023a). The most recent attempt at spatial statistical modeling that considers both SSH and SPD is by More recently, Lessani and Li (2024), who developed the Similarity and Geographically Weighted Regression (SGWR) model, which combines distancebased and similarity and geographically weighted regression model. This new model integrates distance weights and similarity weights to address the based weights to overcome limitations of traditional geographically weighted modelingmethods that address only considers spatial dependency. These studies focused on specific issues such as spatial interpolation, regression, and extreme values. Although these models effectively address the combination of both SSH and SPD, there is currently a lack of a universal spatial statistics tool similar to Focal Statistics and Zonal Statistics. This study aims to develop a spatial statistical model, termed the Focal-Zonal Mixed Statistics, within the framework of GIS spatial statistics. The newly developed toolbox, FZStats v1.0, integrates traditional Focal Statistics and Zonal Statistics, as well as Focal-Zonal Mixed Statistics. In terms of algorithm design, we employ multiprocessing and batch processing techniques, which promise to enhance operational efficiency and user experience. We believe that the FZStats v1.0 toolbox, especially the newly proposed Focal-Zonal Mixed Statistics, has the potential to offer methods and tools to better understand and address SSH and

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SPD issues.

Although these methods successfully integrate SSH and SPD in specific tasks such as interpolation and regression, there is still no general-purpose GIS toolbox comparable to Focal and Zonal Statistics within standard GIS workflows. To fill this gap, this study presents FZStats v1.0, which unifies traditional Zonal Statistics and Focal Statistics with the novel Focal–Zonal Mixed Statistics model. Leveraging multiprocessing and batch-processing capabilities, FZStats v1.0 improves computational efficiency and optimizes usability. Moreover, from a logical perspective, Focal–Zonal Mixed Statistics can be viewed as a generalization of the two traditional approaches. Specifically, when the moving window covers—or substantially exceeds—the entire study area (i.e., window size $\rightarrow \infty$), the method converges to Zonal Statistics, effectively addressing SSH. Conversely, when only a single zone is defined, it simplifies to Focal Statistics, capturing SPD. In the more common and complex scenarios where both SSH and SPD coexist, only the mixed approach is capable of simultaneously accounting for both characteristics. Consequently, FZStats v1.0 is positioned to function as a comprehensive analytical framework for spatial studies necessitating simultaneous evaluation of SSH and SPD parameters across diverse application domains.

2 Models

2.1 Focal Statistics model

The modeling of Focal Statistics method addresses spatial positional dependence by computing summary statistics within a defined neighborhood around each raster cell. The implementation involves three functional methodsmain steps: (1) defining the neighborhood window,—specifying its shape (e.g., square, circular, elliptical) and size; (2) identifying the neighboring cells—located—locating all raster cells—within the neighborhood, of the focal cell; and (3) calculating the neighborhood statisticscomputing statistics—applying a selected statistical function (e.g., mean, sum, minimum, maximum) to the identified neighboring cells and

179 <u>assigning the result to the focal cell</u>.

2.1.1 Defining the neighborhood window

Defining the neighborhood window is a <u>crucial prerequisite for fundamental step in Focal</u>
Statistics. There are This step involves specifying two <u>key parameters to define:</u> the neighborhood window: its <u>window's shape</u> and size. These <u>can be adjusted based on parameters should be determined according to the spatial characteristics of the data and the <u>research</u> objectives of the research. Commonly used shapes. Common shape options include circular, square, and rectangular, while the <u>window</u> size is typically <u>specified in terms of defined by the number of cells.</u></u>

Formally, let *NW* denote the neighborhood window, the following expression can be obtained.

$$NW = f(Shape, Size) \tag{1}$$

where f(.) represents the function used to characterize the To implement these neighborhood windows in a computational framework, we developed three distinct each corresponding to a different geometric shape: rectangular, circular, and elliptical. These window classes are outlined in Listing 1.

```
class KDGeoRectNbhWindow:
           def __init__(self, height: int, width: int):
               self.height = height
               self.width = width
               self.mask_matrix = self._generate_mask_matrix()
           def _generate_mask_matrix(self):...
      class KDGeoCircleNbhWindow:
           def __init__(self, radius: int):
               self.radius = radius
               self.mask_matrix = self._generate_mask_matrix()
           def _generate_mask_matrix(self):...
      class KDGeoEllipseNbhWindow:
           def __init__(self, semi_major_axis: int, axis_ratio: float, azimuth: float):
               self.semi_major_axis = semi_major_axis
               self.axis_ratio = axis_ratio
               self.azimuth = azimuth
               self.mask_matrix = self._generate_mask_matrix()
           def _generate_mask_matrix(self):...
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      Listing 1. Code fragment for the three types of neighborhood window, Shape refers to the geometric
      configuration of the classes: the rectangular window, while Size specifies class
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      (KDGeoRectNbhWindow), the circular window class (KDGeoCircleNbhWindow), and the elliptical window
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      class (KDGeoEllipseNbhWindow).
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           The mathematical essence of a neighborhood window lies in its formal specification of a
      spatial domain of influence, which is typically discretized as a two-dimensional binary mask
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      matrix. This matrix defines the inclusion of neighboring cells within a fixed spatial extent-
      centered on a focal cell. Specifically, it indicates whether each cell in the local neighborhood
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      should be considered for subsequent analysis or computation. The matrix can be formally
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      expressed as:
           NM_{cx,cy}(x,y) = \begin{cases} 1 & \text{if } (x,y) \in \Omega_W \\ 0 & \text{otherwise} \end{cases}
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                                                                                           (1)
      where \Omega_W denotes the neighborhood spatial domain centered on cell (cx, cy), whose
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shown in Listing 1, the <u>generate mask matrix</u> method implemented in each window class is responsible for generating the neighborhood mask matrix according to the specified window parameters (e.g., height, width, radius).

2.1.2 Identifying cells within the neighborhood

Once After the mathematical formulation of the neighborhood window is determined, established (as defined in Eq. (1)), the spatial sliding window technique can be used employed to identify the cells located within the predefined neighborhoods defined by the neighborhood window centered around given cells on each focal cell for localized analysis (Hyndman and Fan, 1996). For each current location Cell(i,j), a given focal cell located at position (i,j), the effective neighborhood cell set can be obtained through the following two computational stages.

(1) Alignment of the neighborhood can be expressed as: mask matrix

Nbh(To ensure accurate spatial correspondence, the geometric center of the neighborhood mask matrix $NM \in \{0, 1\}^{m \times n}$ is aligned with the focal cell located at (i, j) on the raster grid. A mapping is then established from each element in the mask matrix to its corresponding location in the raster data domain. Let the center of the mask matrix be located at (cx, cy), and let (u, v) denote the row and column offsets from the center. Then, the mapping from mask coordinates to raster coordinates is defined as:

$$(x,y) = (i + u,j) = nbh(Cell(i,j), NW) + v)$$

228 (2)

where i and j denote (x,y) denotes the row and column number coordinate of eurrenta neighboring cell at location (i,j), respectively; nbh(.) is in the function for determining raster grid, derived from the neighborhood of Cell(i,j), and NW represents relative offset (u,v) with respect to the focal cell. This mapping ensures that the neighborhood window is precisely

233 <u>aligns with the focal cell</u>.

Then cells located within Nbh(i, j) form a cell set, which can be described as follows:

CS_F(2) Identification of the valid neighborhood cell set

To handle boundary effects when the neighborhood window extends beyond the raster

extent, a boundary-clipping strategy is adopted. That is, only the cells that are entirely located

within the raster data domain Ω_D are retained. The valid neighborhood cell set $C_{F_valid}(i,j)$

239 is defined as:

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 $\mathbf{C}_{F\ valid}(i,j) =$

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$$\{Cell(i^{\iota}, j^{\iota}) \in \mathbf{R}_{\psi} \mid is_in_nbh(Cell(i^{\iota}, j^{\iota}), Nbh(i, j)) == TRUE\}\{(x, y) \in \Omega_D \mid \mathbf{NM}_{cx, cy}(x, y) = 1\}$$

242 _____ (3)

where $is_in_nbh(.)$ — $NM_{cx,cy}(x,y) \in \{0,1\}$ is the indicator function used to identify whether

244 $Cell(i^{t}, j^{t})$ is located within corresponding value in the neighborhood Nbh(i, j); i^{t} and j^{t}

aremask matrix. A value of 1 indicates inclusion as a valid neighbor for the row and column

246 number of the input value raster R_{y} , respectively.

247 — In Eq. (3), the detailed formsubsequent analysis, while a value of is_in_nbh(.) depends

on the shape of the neighborhood window. For example, when the window is circular,

249 *is_in_nbh(.)* can be expressed as:

$$250 \qquad \sqrt{(i^{+}-i)^{2}+(j^{+}-j)^{2}} \leq d \qquad 0$$

251 <u>signifies exclusion</u> (4)

252 where d is the radius of the circular window, i.e. window size, and i and j, and i^{+} and j^{+} are

253 as explained above.

2.1.3 Calculating the focal statistics

Suppose that $ST_{\#}(Type, Set)$ denotes the statistical function of Focal Statistics, and Type

and Set are for the statistical parameter and the cell set to be processed. At the location of

257 Cell(i,j) and under the Focal Statistics model, Set can be specified as $CS_{\mathcal{F}}(i,j)$. Then the

output of the Focal Statistics for Cell(i, j) can be expressed as:

 $O_{\mathcal{F}}(i,j) = ST_{\mathcal{F}}(Type, CS_{\mathcal{F}}(i,j)) \tag{5}$

260 Expressed in terms of raster layer operations, Eq. (5) can be further formulated as:

- $R_{V-out} = Focal_Statistics(R_{v}, NW, Type)$ (6)
- 262 where R_{ii} and $R_{i',out}$ represent the input value raster and the output raster for Focal Statistics,
- 263 respectively, while NW and Type denote the functions for neighborhood window and
- 264 statistical type in that order.

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- 265 After identifying the valid neighborhood cells, their corresponding values are retrieved from
- the raster dataset and organized into a two-dimensional array. Based on these values, statistical
- 267 <u>measures such as mean, percentiles, and other user-defined metrics can be computed. The</u>
- resulting statistic is then assigned to the corresponding position in the output raster.
- 269 This procedure can be implemented through a function that obtains the neighborhood mask
- 270 matrix, identifies valid neighborhood values for the focal cell, and computes the specified
- 271 <u>statistic. Listing 2 presents a representative implementation of this workflow.</u>
- The computation is performed for every cell in the input raster, and the resulting values
- are written to the output raster, producing the final focal statistics result.

```
def calculate_focal_statistics_result(
    nbh_window_mask: np.ndarray,
    data_arr: np.ndarray,
    data_align_pos: Tuple[int, int],
    stats_parameters_list: List[str]
) -> float:
    # Extract neighborhood mask and data centered at the target position
    cur_nbh_mask, cur_nbh_data = calculate_current_nbh(nbh_window_mask, data_arr, data_align_pos)

# Apply the mask to filter out invalid values
    valid_value_arr = cur_nbh_data[cur_nbh_mask]

# Delegate the statistical computation to the external function
    return calculate_statistics(valid_value_arr, stats_parameters_list)
```

Listing 2. Python function *calculate focal statistics result* for computing focal statistics. The function identifies valid values from a neighborhood centered at the focal cell, filters them using a predefined mask, and then calculates the specified statistics.

2.2 Zonal Statistics model

Unlike Focal Statistics, which require only a operate solely on a single value raster as input, Zonal Statistics require requires two input raster layers: one as thea value raster and the other as thea zone raster. The zone raster defines the shapespatial configuration and distribution categorical labels of the zones, and where each cell can only belong assigned to a single exactly one zone. Zonal Statistics calculates the statistics computes summary metrics (e.g., mean, sum, minimum, maximum) for each zone based on by summarizing the values of the corresponding cells from in the value raster, and the calculated. The resulting statistic is then uniformly assigned as the output value for to all cells within the that zone. Finally, the output values of different After all zones are assembled into the processed, the individual results are combined to generate the final output raster.

The implementation of Zonal Statistics modelingtypically involves two functional methods, which are forprimary steps: (1) identifying the set of cells in the value raster by corresponding to each zone based on the zone raster, and (2) calculating zonal summary statistics respectively across those cell values within each zone.

2.2.1 Identifying cells in the value raster falling into each zone

- In Zonal Statistics, spatial overlay analysis can be used is employed to find the zone code

 for associate each cell in the value raster with a specific zone, as defined by a corresponding
- 296 zone raster (Hyndman and Fan, 1996):
- $Z_{k}(i^{\perp}, j^{\perp}) = Zone(Cell(i^{\perp}, j^{\perp}))$. This process maps each cell in the
- 298 <u>value raster to its corresponding</u> (7)
- where $Z_{k}(i^{t},j^{t})$ represents the zone code at location (i^{t},j^{t}) , and Zone(.) is the function that
- returns the zone code for the value raster cell at location (i^{\prime}, j^{\prime}) .
- For a given zone Z_k , the corresponding based on spatial alignment. Based on this mapping,
- cells in the value raster form a cell are grouped according to their zone membership, resulting

in a set $CS_{\mathcal{Z}}(Z_{\mathcal{K}})$, which can be expressed as: of raster cells for each zone.

$$304 \quad CS_{\mathcal{Z}}(Z_{\mathcal{R}}) = \{ \quad Cell(i^{\iota}, j^{\iota}) \in \mathbf{R}_{\mathcal{V}} \mid Zone(Cell(i^{\iota}, j^{\iota})) == Z_{\mathcal{K}} \}$$

$$(8)$$

- 305 **2.2.2 Calculating the zonal statistics Zonal Statistics**
- 306 The calculation of statistics for a given zone Z_k can be represented as:

- 308 It is important to note that the calculated statistics are Once the set of raster cells belonging to
- each zone has been identified, a summary statistic is computed based on the corresponding cell
- 310 <u>values. The result is then uniformly assigned to all cells within eachthat zone, and the statistics</u>
- 311 for. After all zones are ultimately processed, the individual zone-level results are mosaicked
- 312 <u>intoto generate</u> the <u>final</u> output raster.
- Using R_{ψ} and R_{Z} to denote the input layers of value raster and zone raster, respectively.
- 314 Zonal Statistics can be expressed as:

$$R_{Z_{\underline{-out}}} = Zonal_Statistics(R_{\psi}, R_{z}, Type)$$
(10)

- where $R_{Z=out}$ represents the output raster, and Type is for the statistic type.
- Listing 3 demonstrates the implementation of this zonal statistics procedure. The
- 318 calculate_zonal_statistics_result function accepts a value raster (data_arr), a zone raster
- 319 (feature_arr), and a list of statistical parameters. For each unique zone code identified in the
- zone raster, the function identifies the corresponding cell values from the value raster, performs
- the specified statistical computation, and assigns the result to all cells within the zone,
- 322 <u>ultimately yielding a complete zonal statistics output raster.</u>

```
def calculate_zonal_statistics_result(
           data_arr: np.ndarray, feature_arr: np.ndarray, stats_parameters_list: List[str]
       ) -> np.ndarray:
           # Initialize the output array with NaNs to represent undefined statistics
           stats_result_arr = np.full_like(data_arr, np.nan)
           # Identify all unique zone codes in the feature array
           zone_code_list = np.unique(feature_arr)
           for code in zone_code_list:
               # Create a boolean mask identifying all pixels belonging to the current zone
               code_mask = (feature_arr == code)
               # Extract the data values corresponding to the current zone
               masked_data_arr = data_arr[code_mask]
               # Compute statistics for the zone
               stats_result = calculate_statistics(masked_data_arr, stats_parameters_list)
               stats_result_arr[code_mask] = stats_result
           return stats_result_arr
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      Listing 3. Python implementation of the zonal statistics computation. The calculate zonal statistics result
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       function computes a specified statistic for each zone defined in the zone raster and assigns the result to all
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       corresponding cells in the output raster.
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       2.3 Focal-Zonal Mixed Statistics
      Similar to Zonal Statistics, Focal-Zonal Mixed Statistics also require operates on two input
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      raster layers, inputs: a value raster and a zone raster. However, this method uniquely integrates
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      spatial and categorical criteria, combining the specific modeling process localized analysis of
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      Focal Statistics with the zone-based constraints of Zonal Statistics. The computation involves
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      the following two functional methods.primary stages:
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      2.3.1 Identifying cells within the neighborhood that belonging to the same zone
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      Actually In this step, the determination selection of the target relevant cells for analysis is
       governed by two criteria, the spatial proximity, as defined by a neighborhood window centered
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      on the focal cell, and zone homogeneity, requiring that all selected cells belong to the same
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       zone as the focal cell.
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For a focal cell located at position (i, j), the valid neighborhood cell set $C_{FZ_valid}(i, j)$

can be defined as:

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$$C_{FZ_valid}(i,j) = \{(x,y) \in \Omega_D \mid NM_{cx,cy}(x,y) = 1 \land Z(x,y) = Z(i,j)\}$$
 (4)

- 341 where $NM_{cx,cy}(x,y) \in \{0,1\}$ is the corresponding value in the neighborhood mask matrix. A
- value of 1 indicates inclusion as a candidate valid neighbor for subsequent analysis, whereas a
- value of 0 indicates that the cell is excluded. Ω_D denotes the spatial domain of the raster dataset,
- 344 (x,y) are the relative positions of candidate neighboring cells, and Z(i,j) is the zone code of
- 345 the focal cell, which serves as the categorical constraint.

2.3.2 Calculating the Focal-Zonal Mixed Statistics combines

- Once the set of valid neighboring cells has been determined based on both the spatial proximity 347 condition from Focal Statistics, and zone membership, the next step is to compute the 348 349 environmental characteristic similarity condition from Zonal Statistics. For Cell(i, j) at desired statistical measures using the current location, if its neighborhood is Nbh(i,j) and 350 its zone code is $Z_k(i,j)$, then its identified cell set consists of all values. For each focal cell, only 351 those neighboring cells that lie within the neighborhood that belong todefined spatial window 352 353 and share the same zone as the cellcode are included in the statistical calculation. This dual constraint ensures that the resulting Focal-Zonal Mixed Statistics. Mathematically, this can be 354 expressed as: reflects localized variation while maintaining consistency within categorical 355 356 spatial units.
- 357 $CS_{F-Z}(i,j) = \{Cell(i^{\iota},j^{\iota}) \in \mathbf{R}_{F} \mid \frac{is_in_nbh(Cell(i^{\iota},j^{\iota}), Nbh(i,j)) == TRUE}{Zone(Cell(i^{\iota},j^{\iota})) == Z_{\kappa}(i,j)} \}$ (11)

2.3.2 Calculating the focal-zonal mixed statistics

Still using TypeListing 4 demonstrates the implementation of the Focal-Zonal Mixed

Statistics procedure. The <u>calculate focal zonal statistics result</u> function computes a localized statistic for a given focal cell by integrating both spatial and zonal constraints. It first

362 identifies the neighborhood data and associated zone codes based on the predefined window mask centered at the target position. Then, it applies a zonal constraint by retaining only those 363 neighboring cells whose zone codes match that of the focal cell. After applying the combined 364 focal-zonal mask, the specified statistic is computed on the resulting valid value set. 365 The computation is performed for every cell in the input raster, where the neighborhood is 366 constrained both spatially and categorically. The resulting values are written to represent the 367 statistical type, the output result of Focal-Zonal Mixed Statistics for the current Cell(i,j) can 368 be expressed as: 369 $O_{F-Z}(i,j) = ST_{F-Z}(Type, CS_{F-Z}(i,j))$ 370 (12)In the form of raster layer operations, Eq. (12) can be further expressed as: 371 $R_{\text{FZ_out}} = Focal_Zonal_Statistics(R_{\text{F}}, R_{\text{Z}}, NW, Type)$ (13) 372 where R_{x} , R_{z} , and R_{FZ_out} represent the value raster, zone raster, and output raster for 373 producing the final Focal-Zonal Mixed Statistics, respectively; NW is the neighborhood 374 window, and Type is for statistical parameter result. 375

```
def calculate_focal_zonal_statistics_result(
           nbh_window_mask: np.ndarray,
           data_arr: np.ndarray,
           feature_arr: np.ndarray,
           data_align_pos: Tuple[int, int],
           stats_parameters_list: List[str]
       ) -> float:
           # Extract neighborhood mask and data centered at the target center position
           cur_nbh_mask, cur_nbh_data = calculate_current_nbh(nbh_window_mask, data_arr, data_align_pos)
           # Extract the environmental feature values over the same neighborhood window
           _, cur_nbh_feature = calculate_current_nbh(nbh_window_mask, feature_arr, data_align_pos)
           # Retrieve the environmental feature value at the center pixel
           cur_feature = feature_arr[data_align_pos]
           # Create a mask for pixels in the neighborhood that match the center's feature value
           cur_feature_mask = (cur_nbh_feature == cur_feature)
           # Combine the neighborhood shape mask with the feature (zonal) mask
           fz_mask = cur_nbh_mask & cur_feature_mask
           # Filter data values using the combined focal-zonal mask
           valid_value_arr = cur_nbh_data[fz_mask]
           # Compute statistics only on valid data values
           return calculate_statistics(valid_value_arr, stats_parameters_list)
376
```

- Listing 4. Python implementation of the Focal-Zonal Mixed Statistics computation. The function filters
- 378 neighborhood cells based on both spatial proximity and zone code consistency, then calculates a user-
- 379 <u>specified statistic on the resulting valid subset.</u>
- 380 **3 Module design**
- 3.1 Modeling process for Focal-Zonal Mixed Statistics
- The flowchart detailed modeling process for the newly proposed Focal-Zonal Mixed Statistics
- is presented in Fig. 1, and the detailed modeling process is described as follows.

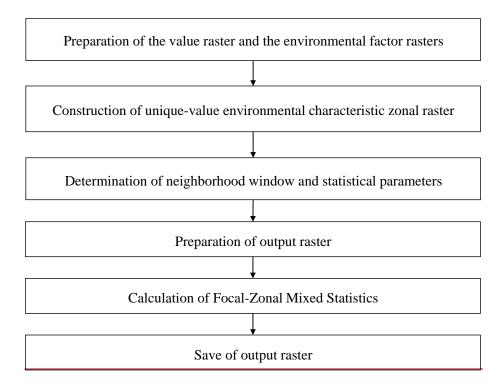


Figure 1. Flowchart for the modeling of Focal-Zonal Mixed Statistics

(1) Preparation of the value raster and the environmental factor rasters

This initial step involves collecting and preprocessing the spatial datadatasets required for the analysis. The value raster typically represents the primary variable of interest, i.e., the target layer,—such as temperature, pollution levels, or vegetation indices. Environmental The environmental factor rasters include various influencing factors, such as characterize variables that potentially influence the spatial heterogeneity of the target variable, including elevation, slope, land cover, and other relevant geographical features that may contribute to the heterogeneous distribution of the target layer, or ecological attributes. Preprocessing methods mayprocedures typically include resampling, reprojecting reprojection, and normalizing the datanormalization to ensure consistency and compatibility among the that all raster layers, so that they share the same a consistent spatial extent, resolution, and coordinate reference system.

(2) Construction of unique-value environmental characteristic zonal raster Unique-Value Environmental Characteristic Zonal Raster (UV-ECZR)

This process can be achieved using the "Reclassify" tool in AreGIS to transform

continuous or categorical environmental factor rasters into discrete classes based on predefined criteria. Subsequently, the UV-ECZR is generated through spatial overlay analysis and uniquevalue encoding. Cells in the UV ECZR that share the same unique value environmental characteristic code (UV-ECC) form a similar environmental unit (SEU). A detailed implementation of this process is described in the following Sect. In this step, environmental factor rasters—whether continuous or categorical—are reclassified into discrete categories using a well-defined discretization scheme. For continuous variables, the classification method should be selected according to the data distribution and research objectives: natural breaks (Jenks) are recommended for datasets exhibiting clear clustering, equal interval classification suits uniformly distributed data, and quantile classification ensures balanced representation across value ranges. For categorical variables, original classes are typically retained unless aggregating categories improves analytical validity. The optimal number of classes, usually between 5 and 8, should balance environmental heterogeneity with adequate sample size within each zone. Classification performance can be evaluated by minimizing within-zone variance, maximizing between-zone variance, and assessing clustering validity through the silhouette coefficient. After reclassification, the final UV-ECZR is produced via spatial overlay analysis, wherein each unique combination of reclassified layers is assigned a Unique-Value Environmental Characteristic Code (UV-ECC). Cells sharing the same UV-ECC form a Similar Environmental Unit (SEU), ensuring that resulting zones capture meaningful ecological thresholds while maintaining sufficient sample sizes for statistical reliability. A detailed methodological workflow for this process is provided in Sect. 3.2.1.

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(3) Determination of neighborhood window and statistical parameters

This process involves defining the neighborhood window and specifying the statistical parameters for Focal-Zonal Mixed Statistics.

This process involves specifying the neighborhood window and specifying the selecting

appropriate statistical parameters for the Focal-Zonal Mixed Statistics. The window size should be selected based on several considerations, including the spatial scale of the studied phenomenon (e.g., local versus regional patterns), the resolution of the input rasters (with coarser resolution favoring larger windows), and computational efficiency (as larger windows significantly increase processing time). The window shape should be chosen according to the nature of spatial anisotropy (elliptical for directional patterns), processing efficiency (rectangular shapes are computationally faster), mitigation of edge effects (circular windows help reduce boundary artifacts), and data characteristics (rectangular for grid-aligned features and circular for isotropic phenomena). The selection of the statistical function should align with the analytical objectives: the mean is suitable for general smoothing and trend detection; the standard deviation is appropriate for identifying variability and anomalies; the minimum and maximum help detect extreme values; percentiles (such as the 90th percentile) support robust threshold analyses; and the sum is useful for aggregation tasks.

(4) Preparation of output raster

This step involves ereatinggenerating an output raster withthat matches the same input rasters in terms of spatial extent, resolution, and coordinate reference system as the input rasters.

This to ensure seamless spatial alignment. The output raster will serves as a container to store the results of the Focal—Zonal Mixed Statistics ealculations computations. Before processing, the output raster is typically initialized with null values (e.g., NoData or NaN) to indicate that no computation has yet been performed. As the computation proceeds, each computed statistic is written into the output raster at the spatial location corresponding to the focal cell.

(5) Calculation of the statistics

In this step, the moving window technique is appliedemployed to locatesystematically traverse each current focal cell and its local window.across the study area. For each current focal cell, identify theits local neighborhood cells is first determined based on the defined predefined

neighborhood window parameters (refer to Sect. 2.1.1). Within this neighborhood, isolate the cells withinbelonging to the same SEU as the eurrentfocal cell. Subsequently, calculate the are identified by comparing their UV-ECC values. The specified statistic for these cells in the statistical measure is then calculated using the corresponding values from the value raster that correspond to those isolated cells for the selected cells. The computed statistic is assigned to the focal cell's position in the output raster. This procedure is repeated iteratively for all focal cells until the output layer is fully generated.

(6) Save of output raster

Write the statistical result to each corresponding cell in the output raster one at a time, and save the raster file after all cells have been processed.

The core algorithm involved in the above steps is described in the following section.

After the computation is complete for all focal cells, the finalized output raster is written to disk. After all cells have been iteratively processed, the complete output raster is finalized and saved to disk. Ensuring proper saving procedures, such as specifying an appropriate file format (e.g., GeoTIFF) and maintaining consistent georeferencing information, is essential to preserve data integrity and facilitate subsequent spatial analyses.

3.2 Core algorithm design for Focal-Zonal Mixed Statistics

3.2.1 Algorithm design for the UV-ECZR construction

Assume that there are p continuous environmental variables, i.e., E_{\pm} denoted as $\{E_1, E_2, ..., E_p, \text{ with }\}$, and their corresponding reclassified variables being CE_{\pm} are $\{CE_1, CE_2, ..., CE_p, \}$. The number of categories for CE_q is denoted as S_q , and the required digit lengths of these categories are denoted as $S_1, S_2, ..., S_p$ and length $D_1, D_2, ..., D_p$, respectively. The method for calculating the digit lengths of the categories is as follows D_q is computed as: $D_q = |\lg S_q| + 1$

- 475 (14<u>(5</u>)
- where \lg denotes the logarithm with base 10, [.] represents the floor function, and q=
- 1, 2, ..., p. The <u>categories category values</u> for the q-theach environmental variable <u>should must</u>
- be a positive integer integers, and the value range of cell value infor the reclassified raster (CE_g)
- 479 can be expressed as CE_q is [1, S_q]. It is necessary to prepend a sufficient number of "0"s to
- 480 ensure the code has a consistent digit length of D_{q} .
- 481 Then, the UV-ECCThus, each pixel at location (i,j) in the raster can be defined
- 482 <u>asrepresented by the vector of its p_reclassified environmental category values:</u>

483
$$CE(i,j) = (CE_1(i,j), CE_2(i,j), \dots, CE_p(i,j))$$
 (6)

$$484 \quad UV - ECC \quad (i,j) = 1 \underbrace{\overline{X} \cdot \overline{X}}_{D_{\overline{x}}} \underbrace{\overline{X} \cdot \overline{X}}_{D_{\overline{x}}} \underbrace{\overline{X} \cdot \overline{X}}_{D_{\overline{y}}} \underbrace{\overline{X} \cdot \overline{X}}_{D_{\overline{y}}} \underbrace{\overline{X} \cdot \overline{X}}_{D_{\overline{y}}}$$
(15)

- where $X \rightarrow X$ represents the each component $CE_q(i,j)$ is the integer category code of
- 486 CE_q the p-th environmental variable at location (i,j), D_q is obtained through Eq. (14). To
- 487 keep the consistency in the UV-ECC format, it pixel (i, j).
- 488 The UV-ECC at pixel (i, j) is necessary to prepend defined as a sufficient number of "0"s
- 489 to ensure unique scalar encoding of the vector $\mathbf{CE}(i,j)$. One efficient way to construct this
- 490 <u>code is by decimal digit length of category code equals D_{q} concatenation:</u>

- 492 (7)
- 493 the form of raster calculator, the UV-ECZR can be expressed as:

$$494 \qquad UV - ECZR = CE_{\pm} \cup CE_{\pm} \cup \dots \cup CE_{p} \tag{16}$$

- 495 where U represents the spatial overlay.
- Based on the framework of raster map algebra, the UV-ECZR is constructed through a
- spatial overlay operation applied to the *p* reclassified environmental variable layers. This

498 process corresponds to a local operation in raster algebra, where the categorical values from each layer are combined on a cell-by-cell basis to generate a multi-dimensional representation. 499 A more realistic and pertinent code sample is provided in Listing 5. 500 import os import arcpy feature_dir = r"E:\rn\paper\p1\A_data\f_z\L_20230928\feature" # List of preclassified environmental variable layers (raster files) ce_layers = ["slope_rc9.tif", "aspect_rc9.tif"] # Read the environmental variable layers into a list of Raster objects ce_rasters = [arcpy.sa.Raster(raster) for raster in ce_layers] # Perform a cell-by-cell overlay operation (local operation in raster algebra) uv_eczr_raster = ce_rasters[0] for raster in ce_rasters[1:]: uv_eczr_raster += raster # Save the resulting UV-ECZR (multi-dimensional raster) uv_eczr_path = os.path.join(feature_dir, "slope_rc9_aspect_rc9.tif") uv_eczr_raster.save(uv_eczr_path) 501 Listing 5. Python implementation of UV-ECZR generation using arcpy-based raster map algebra. Each input 502 503 raster layer represents a reclassified environmental variable (e.g., slope or aspect), and the local overlay 504 operation combines their category codes to produce a unique zone identifier for each pixel. 3.2.2 Algorithm design for determining the valid range for statistics under the sliding 505 506 window technique A rectangular windows, which alignsalign with the rowsrow and 507 columns column structure of raster data and is both easy and efficient to implement, is 508 commonly, are widely used in the sliding window technique operations due to their simplicity 509 510 and computational efficiency. However, its drawback is also evident: the grid-cells located at 511 the four corners are much significantly farther from the current location focal cell than those on

the horizontal and vertical axes (Zhang et al., 2016a). Despite this, rectangular windows remain

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one of among the most popular forms of spatial sliding windows. commonly employed window shapes.

In this study, we consider <u>not only</u> rectangular windows <u>along withbut also</u> circular and elliptical <u>windows.window shapes</u>. Since a circle is a special <u>formcase</u> of an ellipse, <u>we use</u> the ellipse <u>is used</u> as <u>ana generalized</u> example to illustrate the algorithm <u>design</u> for determining the valid range <u>of cells</u> for statistics under the sliding window technique in <u>the context of Focal—</u> Zonal Mixed Statistics.

(1) Mask matrix for elliptical window

An elliptical window is defined by three key parameters: the length of major axis, the ratio of the minor axis to the major axis, and the deflection angle of major axis. Let (x_0, y_0) represent the center of the ellipse, i.e., the current location, a denotes the semi-major axis length, r be the minor-to-major axis ratio, and θ be the deflection angle. Then the elliptical window can be mathematically expressed as:

$$Ellipse((x_0, y_0), a, r, \theta) = \frac{[(x - x_0)\cos\theta + (y - y_0)\sin\theta]^2}{a^2} + \frac{[-(x - x_0)\sin\theta + (y - y_0)\cos\theta]^2}{(ra)^2} - \frac{[-(x - x_0)\sin\theta + (y - y_0)\cos\theta]^2}{(ra)^2}$$

527 (17(8)

Based on Eq. (158), the bounding box of the elliptical window can be represented as $BBox_{ellipse}(minX, maxX, minY, maxY), \text{ where } minX, maxX, minY, maxY \text{ are as follows:}$

530
$$\begin{cases} minX, maxX = x_0 \pm \sqrt{\frac{4CF}{B^2 - 4AC}} \\ minY, maxY = y_0 \pm \sqrt{\frac{4AF}{B^2 - 4AC}} \end{cases}$$

531 (18<u>(9)</u>)

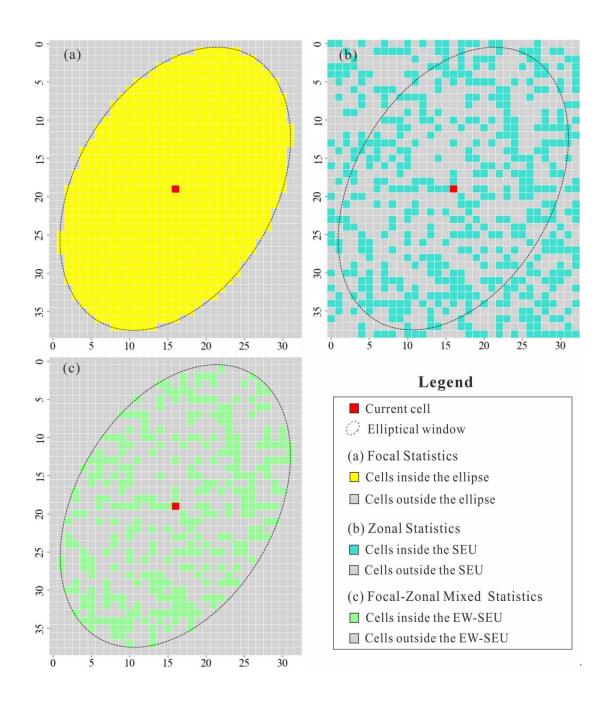
532 herewhere,

$$\begin{cases}
A = a^{2} (\sin^{2} \theta + r^{2} \cos^{2} \theta) \\
B = 2a^{2} (r^{2} - 1) \sin \theta \cos \theta \\
C = a^{2} (\cos^{2} \theta + r^{2} \sin^{2} \theta) \\
F = -\frac{1}{2} (Dx_{0} + Ey_{0}) - r^{2} a^{4}
\end{cases}$$

534 (19(10)

The bounding box $BBox_{ellipse}$ provides a simplified and direct spatial reference for constructing a Boolean mask matrix for the elliptical window, i.e., $Matrix_{Ellipse_mask}$, where cells inside and outside the $BBox_{ellipse}$ are assigned values of "True" and "False", respectively. In Focal Statistics, this <u>binary</u> mask is used directly to <u>define identify</u> the <u>area of interest valid neighborhood cells</u> for <u>statistics</u>, <u>statistical operations</u> (see Fig. <u>2a.1a</u>).





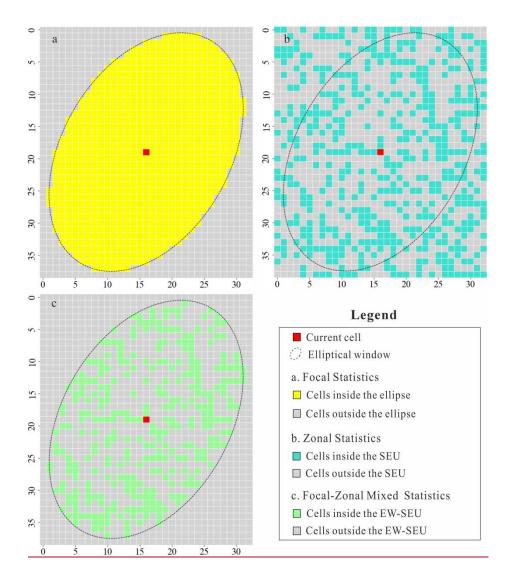


Figure 21. Heatmaps for the Boolean mask matrix: (a) the elliptical window of Focal Statistics, (b) the similar environmental unit (SEU) of Zonal Statistics, and (c) the elliptical window similar environmental unit (EW-SEU) of Focal-Zonal Mixed Statistics.

(2) Mask matrix for similar environment in the bounding box

SEU is the basic object of Zonal Statistics. In Focal-Zonal Mixed Statistics, for the current cell, the elliptical window similar environmental unit (EW-SEU) is established according to the environmental characteristic code within the initial neighborhood window defined by the bounding box. Using $Matrix_{Similarity_mask}$ to represent this unit, cells with the same environmental characteristic code as the current cell are assigned a value of "True", while others are assigned a value of "False", as shown in Fig. 2b1b.

(3) Mask matrix for similar environment in the elliptical window

The matrices of steps (1) and (2) shares the same dimensions, and thus the similar environment mask matrix for the current cell in the elliptical window can be constructed using a logical "AND" operation between these two matrices, as expressed in the following equation:

 $Matrix_{E_S_mask} = Matrix_{Similarity_mask} \land Matrix_{Ellipse_mask} \qquad ---$

558 (20(11)

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- where Λ denotes the logical "AND" operator. $Matrix_{E_S_mask}$ serves as the basis for
- determining the valid range for Focal-Zonal Mixed Statistics, as illustrated in Fig. 2elc.

3.2.3 Algorithm design for the statistics calculation

- The <u>core</u> algorithm for <u>statistical computation within</u> the <u>statistics calculation is designed as</u>
- 563 <u>followsFocal-Zonal Mixed Statistics framework consists of the following steps:</u>

(1) Determination of valid statistical cells in the value raster

- Using $Matrix_{Value}$ to represent the cell array from the value raster within the bounding
- box defined above, then by performing a bitwise multiplication of $Matrix_{E_S_mask}$ with
- 567 $Matrix_{Value}$, the final valid statistical value matrix $Matrix_{Valid}$ is obtained:

$$Matrix_{Valid} = Matrix_{E_S_mask} \otimes Matrix_{Value} \qquad ---$$

569 (21(12)

574

- 570 where⊗denotes bitwise multiplication. This operation collects cells from the value raster that
- are located within the neighborhood and share the same UV-ECC as the current cell, while
- masking out other cells that could interfere with the statistical results. In $Matrix_{Valid}$, the
- 573 masked cells can be represented with "NaN".

(2) Design of the calculation function for the statistics

- Taking $Matrix_{Valid}$ as the final input, the calculation functions for Focal-Zonal Mixed
- 576 Statistics can be designed based on scientific computing tools such as NumPy. This library
- 577 provides a range of statistical methods, including minimum, maximum, mean, standard
- deviation, percentiles, and more. For instance, the "numpy.nanmax()" method can ignore "NaN"

values and return the maximum value of $Matrix_{Valid}$, while the "numpy.nanpercentile()" method, also ignoring "NaN" values, calculates the n-th percentile of $Matrix_{Valid}$.

3.3 User interface design

The Focal-Zonal Mixed Statistics, along with traditional Zonal Statistics and Focal Statistics, are included in the newly developed toolbox, FZStats v1.0, using Python3 and QT5. The user interface is organized into three tabs, each dedicated to one of the three methods, allowing users to switch among them (see Fig. 32). Taking the tab for Focal-Zonal Mixed Statistics as an example, the interface is divided into four main sections, and the detailed description of the user interface design is given as follows.

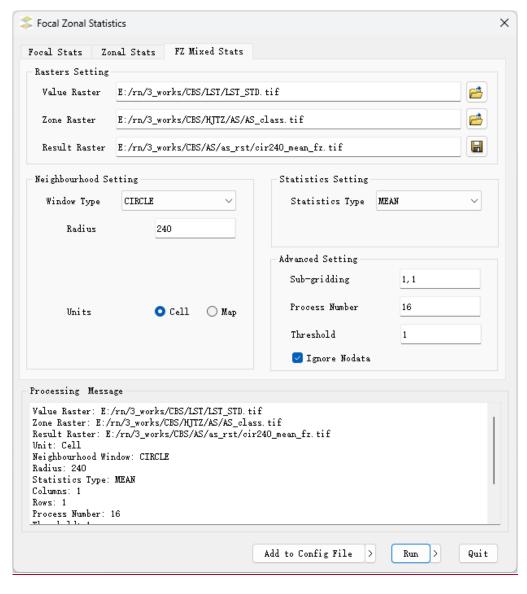


Figure 2. User interface design of FZStats v1.0

(1) Input and output design

Users can selectload the value raster and UV-ECZR <u>layers</u> as <u>input data from their</u> datasets.<u>inputs</u>. Additionally, they can specify the output path and filename for the <u>resultingresult</u> raster <u>datacan be specified</u>.

(2) Neighborhood window design

Users can <u>configuredefine</u> the shape (e.g., rectangular, circular, elliptical) and <u>and size</u> (e.g., number of cells or spatial units) of the neighborhood window. For rectangular and circular windows, size is <u>specifiedcontrolled</u> by the half-side length and radius, respectively. Elliptical windows are <u>characterized usingconfigured via</u> three <u>morphological</u> parameters: the length of the major axis, the ratio of the minor axis to the major axis, and the deflection angle of major axis.

(3) Statistical measure design

<u>Users can select a specified statistical measure from the A</u> dropdown menu-<u>allows users</u> to choose from various statistical measures (mean, max, std, etc.). For percentile-<u>calculations</u>, users are required to specify the exact-based statistics, the desired percentile values of interest, such as the value (e.g., 50th, 75th, or 98th-<u>percentiles</u>) must be specified.

(4) Optimization settings

In this section, users can fine-tune various parameters to optimize the calculation performance. Key settings include:

This section presents optimized parameter configurations to enhance computational efficiency:

Chunk processing: <u>Users can divide the input Divide large</u> raster <u>layers</u> into smaller chunks, which can enhance performance by reducing the <u>to manage</u> memory <u>load and making it easier</u> to <u>handle large datasetsusage efficiently</u>.

Parallel processing: Users can configure Specify the number of processors used forto

enable parallel processing to reduce computation time. On computers with higher configurations, increasing the number of processors allows for the utilization of more cores, enabling simultaneous task execution and significantly reducing processing times and reduce runtime on multi-core systems.

Threshold setting: <u>Users can specifyDefine</u> a minimum sample threshold for statistical calculations, which defines the minimum number of cells required for performing the statistical measure. This threshold ensures that the statistical computations are based on a sufficient sample size, thereby enhancing the reliability and robustness of the operations to ensure robust and meaningful results.

Additionally, to further improve multitasking efficiency and achieve a certain degree of automation, a batch processing featuremode is provided in the toolbox.for automation. Users can define parameters in an INI-formatprepare a configuration file (config.ini), which simplifies the process by eliminating repetitive configurations. This feature allows users to set up and execute) to set parameters for multiple tasks in a single operation, supportsruns. This facilitates efficient task management, parameter reuse, and provides a means forerror tracking-errors.

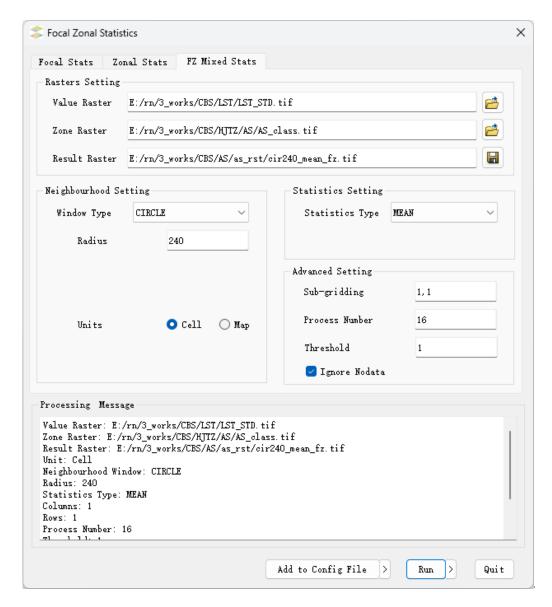


Figure 3. User interface design of FZStats v1.0

4 Experimental study

4.1 Background of the case

Geothermal, like resources, similar to coal, oil, and natural gas, is agre valuable energy mineral resource, and its resources whose development and utilization play a significant role in alleviating energy supply pressure resource and improving the global environment (Huang and Liu, 2010; Goldstein et al., 2011). The most important primary indicator for geothermal resource exploration is the detection of thermal anomalies (Romaguera et al., 2018; Gemitzi et al., 2021). In recent years, with the rapid development advancement of remote sensing, Land Surface

Temperature technologies, land surface temperature (LST) derived from thermal infrared bands has become a key methodparameter for identifying geothermal anomalies. However, LST is influenced by various factors, including not only by geothermal activity but also by environmental factors such as slope, aspect, and surface vegetation cover , among other environmental factors (Tran et al., 2017; Duveiller et al., 2018; Zhao and Duan, 2020).

To effectively extract LST anomalies <u>eaused by directly related to geothermal activity</u>, it is <u>necessaryessential</u> to suppress the <u>influenceconfounding effects</u> of surface environmental variables. Within the analytical framework of the Focal—Zonal Mixed Statistics developed in this study, terrain features are incorporated into environmental zoning, and the spatial sliding window technique is employed to mitigate environmental interference and enhance the <u>abnormal information fromdetection of geothermal activity anomaly signals</u>.

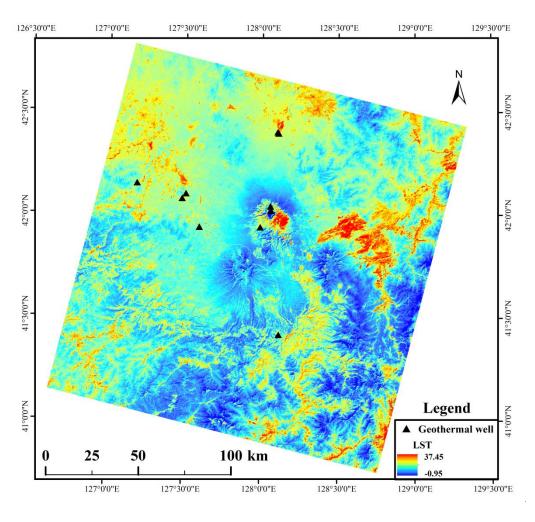
4.2 Data preprocessing

4.2.1 Spatial distribution of LST

In this study, Landsat 8 images imagery (Orbit Number: 116031) observed on September 16, 2013 acquired during the spring, summer, and autumn seasons of 2015, 2019, and 2023, covering the study area, i.e., Changbai Mountain region, were used was utilized for land surface temperature (LST) mapping and geothermal anomaly detection. The selection of multi-temporal images across different seasons and years was intended to robustly validate the effectiveness of the proposed method and to explore the temporal evolution patterns of geothermal anomalies, thereby providing improved support for geothermal exploration in this study. After.

Following standard preprocessing operations such asprocedures, including radiometric calibration and atmospheric correction, the Universal Single-Channel Algorithm (Jiménez-Muñoz et al., 2009, 2014; Zhang et al., 2016b) was employed to retrieve the LST of the study area, as shown in Fig. 4. By comparing Figs. 4 and 5, it can be seen that there is a strong spatial

correlation between LST and terrain factors, especially the slope aspect. Since the local time of the satellite passing over the study area was 10:43 AM, and the solar azimuth angle was 153°, the LST exhibited significantly higher values on the southeast facing slopes than on the northwest-facing slopes applied to retrieve LST across the study area. The resulting LST distributions are illustrated in Fig. 3.



Taking the LST retrieved from the Landsat 8 image acquired on March 20, 2023, as an example, a comparison between Fig. 3 and the terrain information presented in Fig. 4 reveals a strong spatial correlation between LST patterns and topographic factors, particularly slope aspect. Given that the local overpass time of Landsat 8 over the study area was approximately 11:00 AM, with a corresponding solar azimuth angle of 153°, LST values were significantly higher on southeast-facing slopes compared to northwest-facing slopes (Fig. 4a). This highlights the pronounced influence of solar radiation on the spatial variability of LST within

678 the study area.

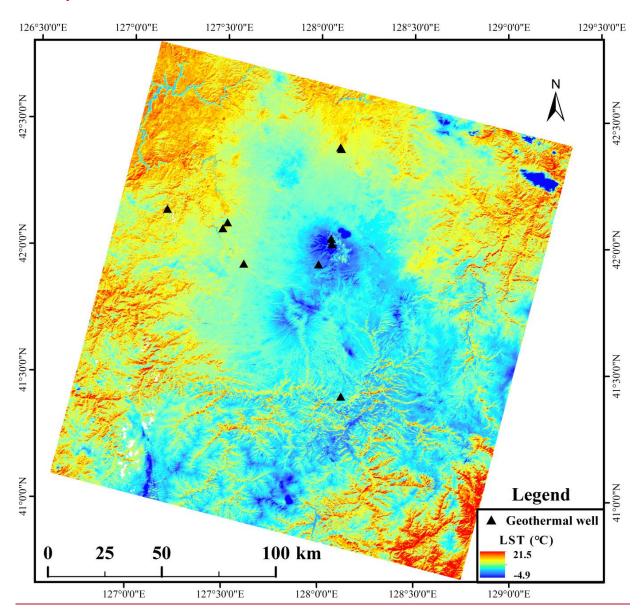
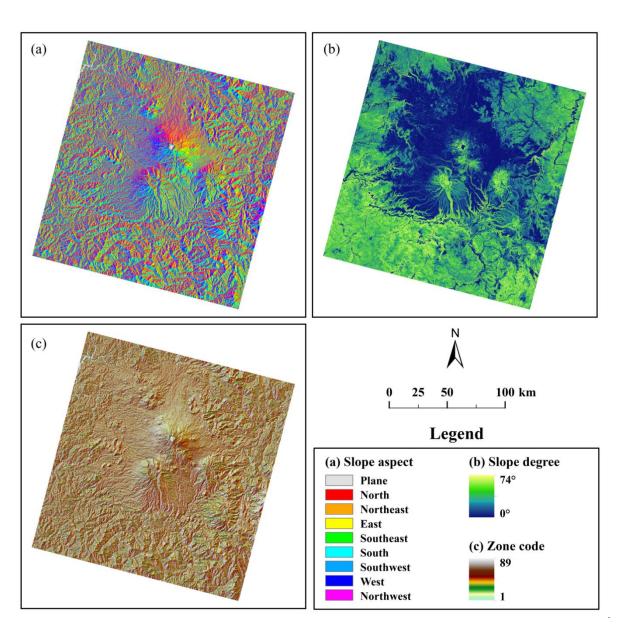


Figure 43. Spatial distribution of land surface temperature (LST) in the study area on March 20, 2023.

4.2.2 Mapping of unique-value environmental characteristic zones

The slopeSlope and aspect were usedselected as the environmental factors to construction construction the UV-ECZR (see Fig. 5a4a and b4b). As previously mentioneddiscussed, these two factors have variables exhibit a strong spatial coupling relationship with LST. Although elevation and vegetation coverage were not directly appliedincluded in the environmental zoning, they process, their variability can be considered similar relatively homogeneous within the defined neighborhood window (Zhang et al., 2019). Therefore Thus, their confounding

effects are indirectly suppressedmitigated. In other words, in the framework of Focal—Zonal Mixed Statistics modeling, sample heterogeneity eaused by arising from long-range spatial variables can be effectively controlled throughby spatial proximity, while that broughtheterogeneity caused by short-range spatial variables ean beis suppressed through environmental similarity.



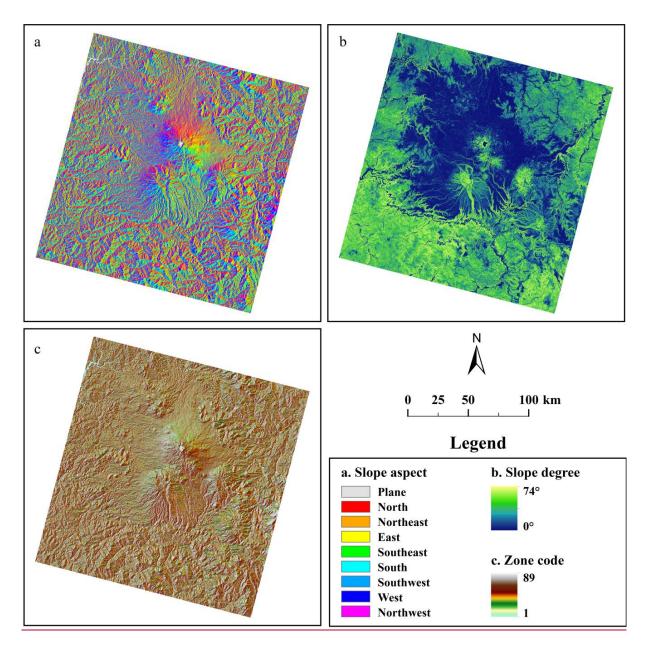


Figure 54. Maps of environmental factors: (a) slopeSlope aspect, (b) Slope degree, and (c) the composite unique value environmental characteristic zonal rasterUnique-Value Environmental Characteristic Zonal Raster (UV-ECZR).

4.3 Enhancement of geothermal anomalies based on Focal-Zonal Mixed Statistics

In mineral prospectivity mapping, standard deviation standardizationnormalization (Z-score transformation) is oftencommonly employed to assist in constructing indicator variables for prospecting anomaly detection (Journel & Huijbregts, 1978; Goovaerts, 1997). This processprocedure involves subtracting the mean from the original value and then dividing the result by the standard deviation. This indicator reveals how many standard deviations the

original, rescaling variables to a uniform range to mitigate scale-dependent biases and enhance comparability of multi-source geochemical data in predictive modeling (Carranza, 2008). The resulting standardized value deviates quantifies the deviation of the original measurement from the mean. The essence of this method—in units of standard deviations. The core principle lies in determining thedefining an appropriate sample range for calculating the local background statistics (e.g., mean and standard deviation, enabling a comparison of the), which ensures meaningful comparisons between the current value against the mean and using the standard deviation to quantify this difference. and its spatial context (Cheng, 2007; Wang et al., 2011). In this study, Focal—Zonal Mixed Statistics was used for this purpose, i.e., defining adopted to define the comparable sample range based on both by simultaneously considering spatial proximity and environmental similarity. Specifically, in this case, the level of LST at for each current location-is, the level of land surface temperature (LST) was assessed within the rangea sample set determined jointly by both the local moving window and the similar terrain features. This approach mitigates method effectively suppresses the influence of factors such as terrain—and, vegetation, thereby producing a and other confounding factors, allowing the resulting LST anomaly distribution map of LST anomalies thatto predominantly reflects reflect geothermal activity. When the current Using a circular moving window is a circle with a radius of 74.2 km, the final enhanced geothermal anomaly map derived from Fig. 3 is shown in Fig. 65.

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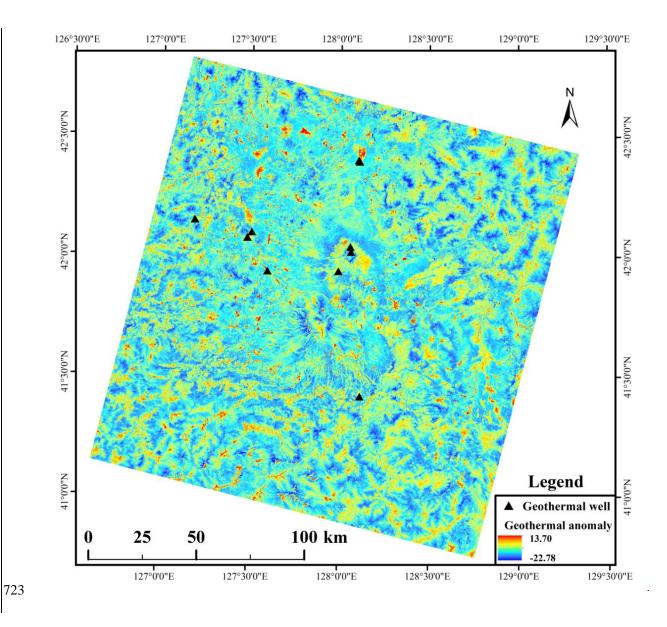
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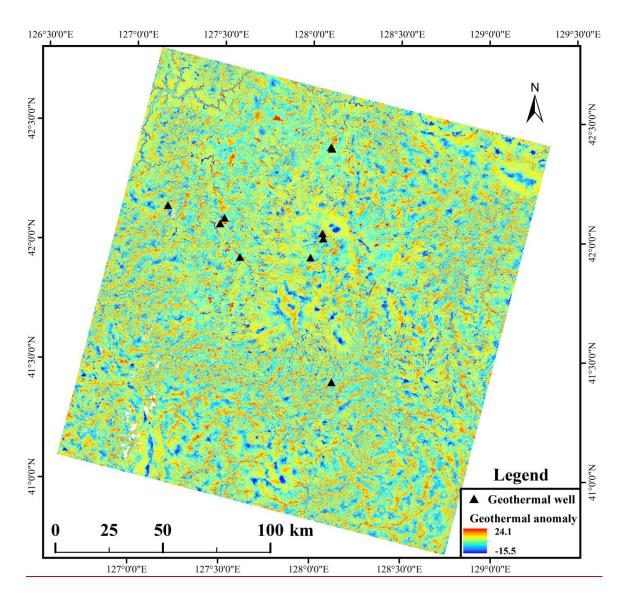


Figure 65. Enhanced geothermal anomaly map based on Focal-Zonal Mixed Statistics with a local window radius of 74.2 km.

Comparing Figs. 5 and 63, it is evident that the LST anomalies enhanced using through Focal-Zonal Mixed Statistics exhibitshow a betterstronger spatial correlation with known geothermal wells (obtained from as referenced by Yan et al., 2017), and their high values indicate known). The higher values in Fig. 5 more effectively highlight these geothermal wells more effectively. Therefore, we have reason to believe, suggesting that the high-value areas with high values in Fig. 6this figure have a higher probabilityan increased likelihood of revealing indicating new geothermal resources.

4.4 Performance Comparison

735	Following the standard deviation normalization approach described above, Zonal Statistics and
736	Focal Statistics were also applied to the LST dataset (Fig. 3) to enhance geothermal anomalies,
737	thereby facilitating comparative evaluation of the models. Specifically, the Receiver Operating
738	Characteristic (ROC) curve was employed to assess the predictive performance of the original
739	LST and the three enhancement indices derived from Focal Statistics, Zonal Statistics, and
740	Focal-Zonal Mixed Statistics.
741	The ROC curve plots the False Positive Rate (FPR) against the True Positive Rate (TPR)
742	(Fawcett, 2006; Hanczar et al., 2010), and the Area Under the Curve (AUC) is used as a
743	quantitative metric for model evaluation. AUC values range from 0.5 to 1, where higher values
744	indicate better predictive accuracy and model performance.
745	The ROC curves for the LST dataset and the three enhancement indices are presented in
746	Fig. 6, where subfigures a-d correspond to the four observation dates: March 20, June 24,
747	September 28, and December 25, 2023. Focal Statistics and Focal–Zonal Mixed Statistics were
748	both implemented using a circular window with a radius of 4.2 km. It is evident that, across all
749	seasons, the enhancement indices derived from the Focal-Zonal Mixed Statistics approach
750	consistently outperform the others. For instance, in Fig. 6a, the AUC value under Focal-Zonal
751	Mixed Statistics reaches 0.734, notably higher than that of Zonal Statistics (0.508), Focal
752	Statistics (0.669), and the original LST (0.474). Although both Zonal Statistics and Focal
753	Statistics demonstrate slight improvements over the raw LST, their enhancement effects remain
754	limited. Furthermore, comparison of Fig. 6a-d indicates that our enhanced model performs best
755	in autumn, as evidenced by the highest AUC value observed in this season.

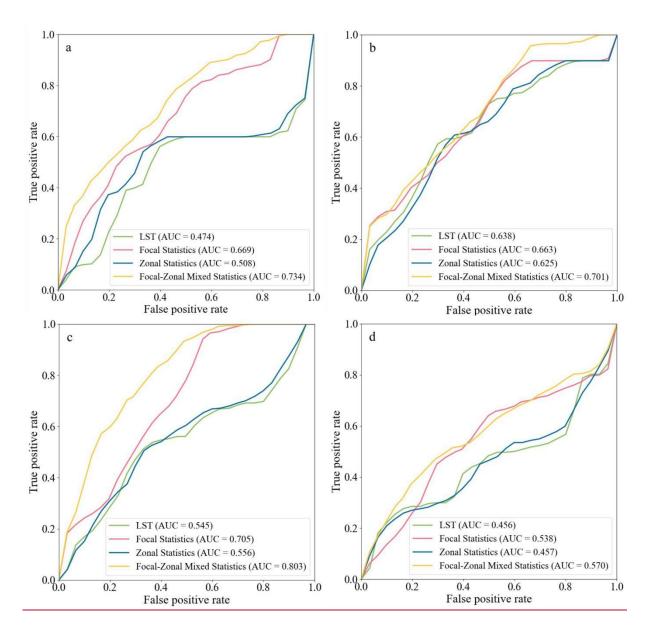


Figure 6. Receiver Operating Characteristic (ROC) curves of the Land Surface Temperature (LST) and its three enhancement indicators derived from Focal Statistics, Zonal Statistics, and Focal—Zonal Mixed Statistics, respectively. A Parameter settings: the local window used for both Focal Statistics and Focal—Zonal Mixed Statistics is a circle with a radius of 4.2 km; the zoning categories used for Zonal Statistics are identical to those employed in Focal—Zonal Mixed Statistics; and a geothermal well represents an area of 0.035 km² surrounding it.

5 Discussion

5.1 Advantages Significance and Necessity of the new statistics New Statistical Method Based on the standard deviation standardization approach described above, we also employed Zonal Statistics and Focal Statistics to enhance geothermal anomalies for further model

comparison. Specifically, the Receiver Operating Characteristic (ROC) curve was used to compare the performance of LST itself and its three enhancement indices in geothermal prospectivity mapping.

The ROC curve is plotted with the False Positive Rate (FPR) and True Positive Rate (TPR) as the x-axis and y-axis, respectively (Fawcett, 2006; Hanczar et al., 2010), and the resulting Area Under Curve (AUC) is used for quantitative evaluation of certain indices or models. AUC values range from [0.5, 1], where higher values indicate better predictive performance and accuracy of the model, and vice versa.

The ROCs of LST and its three enhancement indices obtained by Focal Statistics, Zonal Statistics, and Focal Zonal Mixed Statistics, respectively, are depicted in Fig. 7. It can be observed that the enhancement effect based on Focal Zonal Mixed Statistics is significantly better than that based on the other two models, as the AUC of Focal Zonal Mixed Statistics is 0.731, which is much higher than that of Zonal Statistics (0.638) and Focal Statistics (0.657). Moreover, the AUC values of the latter two are also higher than that of LST, although marginally.

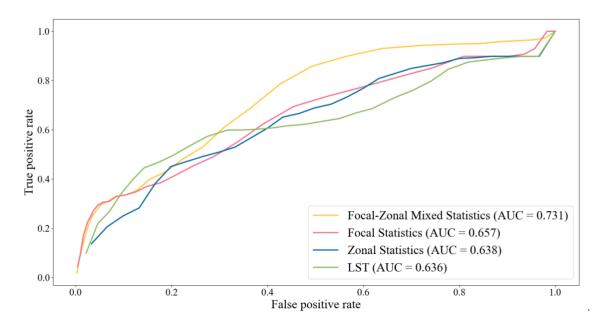


Figure 7. The ROCs of Land Surface Temperature (LST) and its three enhancement indicators obtained by Focal Statistics, Zonal Statistics, and Focal Zonal Mixed Statistics, respectively. Parameter Settings: the local window for Focal Statistics and Focal Zonal Mixed Statistics is a circle with a radius of 7.2 km; the categories

used for Zonal Statistics are the same as those for Focal-Zonal Mixed Statistics; and a geothermal well represents an area of 0.1 km surrounding it. 786 Firstly, from a theoretical standpoint, traditional methods each address only one aspect of spatial 787 variation: Focal Statistics primarily captures SPD, while Zonal Statistics is designed to account 788 for SSH. However, real-world spatial problems often exhibit both characteristics 789 simultaneously. This underscores the theoretical necessity and practical relevance of developing 790 791 the new method—Focal–Zonal Mixed Statistics—which bridges the methodological gap 792 between Focal Statistics and Zonal Statistics. 793 Secondly, from a conceptual perspective, Focal–Zonal Mixed Statistics can be viewed as a generalization of the two conventional approaches. When the moving window encompasses— 794 or far exceeds—the entire study area (i.e., the window size approaches infinity), the method 795 796 converges to Zonal Statistics, effectively capturing stratified heterogeneity. Conversely, when the analysis is confined to a single environmental zone, the method reduces to Focal Statistics, 797 798 thereby focusing on spatial positional dependence. This flexibility enables the new method to seamlessly adapt to different spatial structures. 799 Thirdly, in terms of practical performance (see Fig. 6), although traditional methods show 800 801 some ability to enhance geothermal anomaly detection—for example, Focal Statistics improves AUC values by 3.9% to 41.1% over the original LST—the proposed method demonstrates 802 significantly greater efficacy, with AUC improvements ranging from 9.9% to as high as 54.9%. 803 804 These results clearly highlight the superior performance of Focal–Zonal Mixed Statistics. Finally, regarding broader applicability, although geothermal anomaly enhancement 805 serves as the illustrative case in this study, the utility of the proposed method extends well 806 beyond this specific context. It is particularly well suited for applications requiring both 807 improved sample purity and simultaneous control over SSH and SPD. Potential domains 808 include mineral resource potential evaluation, vegetation restoration potential assessment, 809 cropland productivity analysis, and terrestrial vegetation carbon sink estimation. Furthermore, 810

the method can be employed to assess the spatial variability of target variables under specific environmental constraints, and to evaluate the effectiveness of environmental factors in delineating spatial patterns of interest.

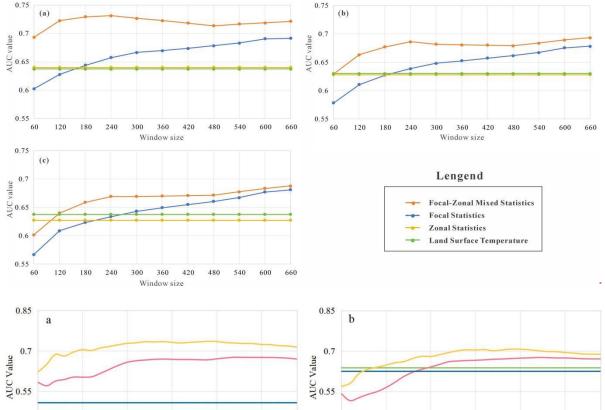
5.2 Robustness of the new method

To ensure that the superior performance of the new model proposed method, as demonstrated in Sect. 5.14.4, is not coincidental due to chance, it is necessary to adjust essential to test its robustness under varying conditions. This involves adjusting key parameters such as the size of the local analysis window-size, the year and the geothermal well-season of image acquisition, and the representative area and conduct assigned to geothermal wells. Through multi-scenario comparison comparative experiments. This will help analyze, the robustness consistency and reliability of the new model'smodel's advantages can be systematically evaluated.

To rigorously assess the robustness of the proposed method, we conducted a series of controlled experiments involving multiple scenarios. Specifically, Landsat imagery from the years 2015, 2019, and 2023 was selected, covering all four seasons—spring, summer, autumn, and winter—for each year. Due to cloud contamination and other data quality issues, some missing seasonal scenes were replaced with imagery from adjacent years and similar months. In addition, two representative areas were defined for individual geothermal wells: 0.0009 km² (equivalent to a single 30 m × 30 m pixel) and 0.035 km². To further test the model's sensitivity to spatial scale, we varied the radius of circular local windows from 0.3 km to 9 km in 0.3 km increments. These selections of years, seasons, neighborhood sizes, and point representativeness were all deliberately designed to evaluate the stability and generalizability of the proposed method relative to the two traditional approaches.

When the representative area for a geothermal well is determined by 0.1km, 0.2km, and 0.3km buffers, respectively defined as a circle with an area of 0.035 km², and imagery from the year 2023 is used for modeling, the AUC values for of the original LST and its enhancement

indices are calculated. These values, _across different seasons and a range of local window sizes. Specifically, circular windows with radii ranging from 0.3 km to 9 km (at 0.3 km intervals) are applied to evaluate model performance. The AUC values obtained through—under these varying seasonal and spatial conditions—across different models—under various local window radii, are _are plotted onin a Cartesian coordinate system, as shownillustrated in Fig. 8.-7.



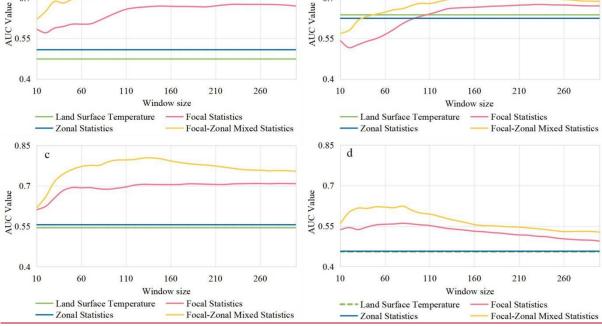


Figure 8. The changes 7. Variations in AUC values with the window size of increasing local window radius (measured in pixel units) for Land Surface Temperature (LST) and its three enhancement indicators obtained

845	by indices derived from Focal Statistics, Zonal Statistics, and Focal-Zonal Mixed Statistics, when a. The
846	geothermal wells are represented as circles with an area of 0.035 km². Panels (a) through (d) correspond to
847	the LST data acquired in the spring, summer, autumn, and winter of 2023, respectively.
848	Appendix Figs. S1 and S2 present the modeling results for the years 2015 and 2019,
849	respectively, under the condition that each geothermal well is represented by a circular area of
850	<u>0.035 km².</u>
851	Appendix Figs. S3 to S5 show the results for the years 2015, 2019, and 2023, respectively,
852	where the representative area for each geothermal well represents circles with a radius of (a) 0.1km,
853	(b) 0.2km, and (e) 0.3km, respectively is defined as a single pixel (30 m × 30 m, i.e., 0.0009 km²).
854	Overall, the two enhancement models incorporating neighborhood windows, i.e.,Focal
855	Statistics and Focal-Zonal Mixed Statistics, perform better than consistently outperform
856	both the Zonal Statistics model and the original, unenhanced LST without enhancement. The
857	relatively poor performance of Zonal Statistics is dueprimarily attributed to the strong spatial
858	variability of LST and the simplicitylimitations of the simple classification scheme used.
859	Additionallyemployed. Moreover, since local windowneighborhood-based methods are
860	<u>inherently</u> sensitive to spatial scale, the <u>performanceeffectiveness</u> of <u>both</u> Focal Statistics and
861	Focal—Zonal Mixed Statistics varies with thechanges in window size.
862	However, regardless of whether the specific modeling configuration—including different
863	years (2015, 2019, or 2023), seasons (spring, summer, autumn, or winter), definitions of the
864	geothermal well representative area is 0.1km, 0.2km, or 0.3km, the performance of (either a
865	single pixel of 0.0009 km² or a circular area of 0.035 km²), and a wide range of local window
866	sizes (radii from 0.3 km to 9 km in 0.3 km intervals)—Focal—Zonal Mixed Statistics
867	consistently surpasses that of delivers superior performance compared to Focal Statistics. This
868	consistent advantage across diverse scenarios and parameter settings clearly demonstrates the
869	robustness and broader applicability of the proposed method.

5.3 Advancements of the Toolbox

The FZStats v1.0 <u>toolbox</u> developed in this study not only integrates traditional Focal Statistics and Zonal Statistics, <u>which deal with __addressing_SPD</u> and SSH, respectively, __but also innovatively implements Focal_Zonal Mixed Statistics <u>based_onby_combining_spatial</u> proximity and environmental similarity, <u>addressing_enabling_simultaneous_handling_of_both_spd_simultaneous_handling_of_both_spd_simultaneous_handling_of_spatial_statistics_statistical_analysis_s.</u>

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A-To enhance its applicability across diverse scenarios and computing environments, the toolbox provides a variety of parameter-setting interfaces are provided to enhance the statistical applicability of the developed toolbox, ensuring it meets the requirements of different application scenarios and computing conditions. In terms of neighborhood window settings, in addition toconfiguration, users can select from rectangular and, circular windows, an, or elliptical window is also available, windows, with the elliptical option allowing users to express the expression of spatial anisotropy in the neighborhood through elliptical adjustable parameters. Regarding statistical parameters measures, the new toolbox supports traditional metrics likesuch as mean, standard deviation, minimum, and maximum-values, as well as calculations for flexible calculation of arbitrary percentiles. To make the best use of to suit specific analytical needs. To optimize memory usage and CPU capabilities, the toolbox computational efficiency, FZStats v1.0 supports both raster data chunk processing and multi-process operation modes, accommodating. This design accommodates different computer memoryhardware capacities and enabling enables efficient parallel processing on multi-core CPUs. Additionally, users can setspecify a minimum cell number of samplescells for valid statistics through the "Threshold" parameter-to avoid, effectively preventing low-statistical-precision and unreliable results due tocaused by insufficient sample size. sizes.

LastlyFinally, to enhanceimprove automation and efficiency in multitasking efficiency, the toolbox providesoffers a batch processing solution. Users can writedefine processing

parameters into an INI-formatwithin a multi-section INI-format configuration file, which avoids thus avoiding repetitive and tedious manual operations. This can not only enable functionality supports one-time parameter setup and, automatic execution of multiple tasks, but support parameter reuse, and error tracing tracking, significantly enhancing operational efficiency and reliability.

6 Conclusions

This study developed the FZStats v1.0 toolbox using Python3 based on Python 3 and QT5. The new toolbox integrates, integrating traditional Focal Statistics, Zonal Statistics, and the newly developed proposed Focal—Zonal Mixed Statistics. We provided detailed algorithmDetailed algorithmic implementations and modeling processes for these methods were presented, and evaluated—their performance inwas evaluated through geothermal anomaly identification.detection experiments. The main conclusions are summarized as follows:

First, the development of the Focal—Zonal Mixed Statistics is essential crucial, as it addresses gaps that the limitations of traditional Focal Statistics and Zonal Statistics cannot fill., providing a unified solution for simultaneously handling SPD and SSH.

Second, FZStats v1.0 offers extensive parameter_setting optionscapabilities, supporting different_flexible configurations of window shapes and types of statistics; simultaneously, by adjustingstatistical measures. Additionally, through adjustable processing parameters, it options such as raster chunking and multi-processing, the toolbox can ensuremaintain efficient performance on computers with varying configurations. across a range of computing environments.

Third, case <u>study</u> analyses <u>showdemonstrate</u> that Focal_Zonal Mixed Statistics significantly enhance <u>the detection of geothermal anomalies compared to <u>conventional</u> Zonal <u>Statistics</u> and Focal Statistics methods, with this advantage <u>beingproving</u> robust <u>across different conditions</u>.</u>

921 In summary, FZStats v1.0 not only innovates contributes theoretical innovation to spatial statistical methods theoretically but also demonstrates powerful exhibits strong functionality 922 and flexibility in practical applications, making it a promising tool in the field of. It holds 923 924 considerable promise for geothermal anomaly identification detection and other areas broader <u>fields</u> requiring <u>integrated</u> spatial statistical solutions. 925 Acknowledgments 926 927 This study benefited from joint financial support by National Natural Science Foundation of China (No. 42071416), 42071416), the New Geochemical Exploration Technology for Shallow-928 929 Covered Landscapes in Desert Gobi and Alpine Steppes (No. 2024ZD1002400) under the Sub-Project "Geochemical Intelligent Prospecting Prediction and Software Development for 930 931 Copper Nickel and Gold Deposits" (No. 2024ZD1002406), and the "CUG Scholar" Scientific Research Founds at China University of Geosciences (Nos. 2022062 & 2024001). 932 933 Code availability. The source code for FZStats v1.0 is available on GitHub at https://github.com/Renna11/FocalZonalStatistics. The latest version of the software can be 934 935 obtained at https://zenodo.org/records/13208114. **Data availability.** The sources of the original data supporting the case study in this paper are as 936 follows: (1) Landsat 8 images used in this research were downloaded from 937 https://earthexplorer.usgs.gov (last accessed: 3 August 2024); (2) Land Surface Temperature 938 939 data can be obtained from http://databank.casearth.cn (last accessed: 3 August 2024); (3) original elevation data used for calculating slope and aspect is from the Shuttle Radar 940 Topography Mission (SRTM) Global 1 Arc-Second Product, provided by NASA, available at 941 https://earthexplorer.usgs.gov (last accessed: 3 August 2024); and (4) geothermal well data is 942 sourced from Yan al. (2017).found 943 et Sample data can be at https://zenodo.org/records/13766015. Readers can refer to the instructions provided in the 944 "README.md" file on the code repository (https://github.com/Renna11/FocalZonalStatistics) 945

- of for guidance on software use, which allows for the reproduction of the case analysis using the
- 947 aforementioned original data.
- 948 Author contributions. DZ and QC conceived the original idea. NR and DZ developed the
- software. NR handled data processing and drafted the manuscript. DZ and QC revised the
- 950 manuscript. All authors read and approved the final manuscript.
- 951 *Competing interests.* The authors declare no competing interests.

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