



| 1  | FZStats v1.0: a raster statistics toolbox for simultaneous management of spatial                     |
|----|--|
| 2  | stratified heterogeneity and positional dependence in Python   |
| 3  |  |
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| 10 | Abstract: Based on the traditional Focal Statistics and Zonal Statistics tools of mainstream         |
| 11 | GIS software, we developed a raster statistics toolbox named FZStats v1.0 using Python3 and          |
| 12 | QT5. The main contributions of this study are as follows. Firstly, the development of a              |
| 13 | specialized spatial analysis toolset designed to comprehensively address stratified                  |
| 14 | heterogeneity, positional dependence, and their combinations, thereby addressing gaps in             |
| 15 | existing Focal and Zonal methods that individually tackle stratified heterogeneity and               |
| 16 | positional dependence problems. Secondly, our toolset features a user-friendly interface and         |
| 17 | structure, integrates both existing and enhanced spatial statistical methods, supports               |
| 18 | multi-processing and batch processing capabilities, and provides users with the flexibility to       |
| 19 | select calculation methods tailored to their computer configurations and application                 |
| 20 | requirements. Thirdly, the newly proposed Focal-Zonal Mixed Statistics method demonstrates           |
| 21 | superior predictive accuracy compared to the traditional Focal Statistics and Zonal Statistics       |
| 22 | methods in geothermal detection, which preliminarily showcases the advantages of this new            |
| 23 | approach. Additionally, we discussed the advantages, robustness, and advancements of the             |
| 24 | Focal-Zonal Mixed Statistics method, concluding that the development of this new method              |
| 25 | and toolset is necessary and holds substantial potential for applications across diverse fields.     |
| 26 | Keywords: Spatial Statistics; Raster Operations; Spatial Heterogeneity; Spatial Dependency;          |
| 27 | Focal/Zonal Statistics.  |





# 28 1 Introduction

The advent of Geographic Information Systems (GIS) marks a milestone in the evolution of 29 geography. As a core function of GIS software, spatial statistics provide powerful methods 30 31 and tools that enable researchers and decision-makers to analyze spatial patterns and associations on the Earth's surface comprehensively and accurately. Spatial heterogeneity and 32 33 positional dependence are two fundamental characteristics to be considered in spatial data processing (Goodchild and Haining, 2004). Correspondingly, Zonal Statistics and Focal 34 Statistics are two essential methods of spatial statistical analysis. The former can be achieved 35 36 through a model that involves partitioning raster data into several zones based on predefined 37 rules or attributes, performing statistical analyses on the raster cells within each zone, and then outputting the results as a mosaic raster layer (Singla and Eldawy, 2018; Haag et al., 38 39 2020; Winsemius and Braaten, 2024). The latter, also known as neighborhood or local window statistics, takes each raster cell as the center and extends a specified range 40 41 surrounding the center to form a local window according to the designated window size; it 42 performs statistical analyses on the raster cells within this window and then outputs the results as a mosaic raster layer (Mathews and Jensen, 2012; Kassawmar et al., 2019; Zhang et al., 43 2021). The calculated statistics for both zonal and focal methods are similar, including the 44 45 mean, maximum, minimum, sum, and so on.

46 Currently, the mainstream GIS software platforms including ArcGIS and QGIS provide 47 tool modules such as Focal Statistics and Zonal Statistics, which have promoted the usage of 48 these two methods. From an application perspective, Zonal Statistics primarily address spatial 49 stratified heterogeneity (SSH), which can be detected by dividing the target variable though 50 environmental characteristic classified variables (Wang et al., 2016; Wang and Xu, 2017; Gao 51 et al., 2022). For instance, the actual or potential growth of vegetation may vary significantly 52 due to different environmental conditions such as slope and aspect (Zhang et al., 2018, 2019;





Xu et al., 2020). With respect to Focal Statistics, it focuses on spatial position dependence (SPD), which can be addressed or at least weaken by introducing the local windows or geographic weights (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 diminish with decreasing distance, indicating that these attributes are dependent on spatial position (Krige and Magri, 1982; Trangmar et al., 1986; Zuo, 2014).

In our real world, SSH and SPD may coexist, with the former exhibiting abrupt changes 60 61 and the latter exhibiting gradual changes. For example, due to variations in land-sea distribution, solar radiation, and altitude, terrestrial vegetation exhibits strong meridional, 62 latitudinal, and vertical zonal distribution patterns respectively (Qiu et al., 2013; Dong et al., 63 64 2019; Eddin and Gall, 2024), which explains the significant SPD in vegetation coverage. Meanwhile, due to the influence of local topography, microclimate, and human activities, the 65 vegetation coverage differences caused by these factors do not entirely manifest as gradual 66 changes. Typical evidence includes phenomena such as vegetation on shady and sunny slopes 67 generally shows SSH (Álvarez-Martínez et al., 2014; Zhang and Zhang, 2022; ) and 68 significant differences between urban and rural landscapes (Zhang et al., 2023b). Furthermore, 69 70 due to differences in formation age, there are significant variations in material across strata, 71 which is a major reason for the SSH of mineral resources distribution (Zhao Pengda, 2006; Zuo, 2020). Subsequently, under the influence of internal and external geological processes, 72 the distribution of mineralization elements often exhibits SPD characteristics (Cheng, 2006, 73 74 2012), and Geostatistics and Kriging methods were developed to explain this phenomenon (Krige, 1951; Goovaerts, 1997; Müller et al., 2022). Therefore, when dealing with problems 75 involving spatial statistics, it is necessary to consider both SSH and SPD simultaneously. 76

77

Some scholars have noted this issue and developed certain improved models in their





respective fields to overcome the challenges posed by solely considering SSH or SPD. 78 Professor Zhu and his group expanded upon traditional spatial interpolation methods, which 79 typically focus solely on spatial dependence, by introducing constraints derived from 80 81 environmental similarity (Zhu et al., 2019). They further proposed the "Third Law of Geography", which states that the more similar the geographic configurations of locations, the 82 83 more similar the values (processes) of the target variable at these locations (Zhu et al., 2018; 84 Zhu et al., 2020). Meanwhile, Professor Zhang and his group enhanced traditional vegetation potential assessment models, which typically only consider similar habitat conditions, by 85 86 incorporating spatial sliding window techniques (Zhang et al., 2019). This development led to 87 a model for assessing vegetation restoration potential based on local windows, simultaneously considering spatial proximity and environmental similarity (Xu et al., 2020; Zhang, 2023a). 88 89 The most recent attempt at spatial statistical modeling that considers both SSH and SPD is by Lessani and Li (2024), who developed similarity and geographically weighted regression 90 91 model. This new model integrates distance weights and similarity weights to address the 92 limitations of traditional geographically weighted modeling that only considers spatial 93 dependency.

These studies focused on specific issues such as spatial interpolation, regression, and 94 95 extreme values. Although these models effectively address the combination of both SSH and 96 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 97 Focal-Zonal Mixed Statistics, within the framework of GIS spatial statistics. The newly 98 99 developed toolbox, FZStats v1.0, integrates traditional Focal Statistics and Zonal Statistics, as 100 well as Focal-Zonal Mixed Statistics. In terms of algorithm design, we employ 101 multiprocessing and batch processing techniques, which promise to enhance operational 102 efficiency and user experience. We believe that the FZStats v1.0 toolbox, especially the newly





- 103 proposed Focal-Zonal Mixed Statistics, has the potential to offer methods and tools to better
- 104 understand and address SSH and SPD issues.
- 105 2 Models

# 106 2.1 Focal Statistics model

- 107 The modeling of Focal Statistics involves three functional methods: (1) defining the
- neighborhood window, (2) identifying the cells located within the neighborhood, and (3)
- 109 calculating the neighborhood statistics.
- 110 2.1.1 Defining the neighborhood window
- Defining the neighborhood window is a crucial prerequisite for Focal Statistics. There are two parameters to define the neighborhood window: its shape and size. These can be adjusted based on the spatial characteristics of the data and the objectives of the research. Commonly used shapes include circular, square, and rectangular, while the size is typically specified in terms of the number of cells.

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

118 
$$NW = f(Shape, Size)$$
 (1)

119 where f(.) represents the function used to characterize the neighborhood window, Shape 120 refers to the geometric configuration of the window, while Size specifies its extent.

# 121 2.1.2 Identifying cells within the neighborhood

Once the neighborhood window is determined, the spatial sliding window technique can be used to identify the cells located within the neighborhoods defined by the neighborhood window centered around given cells (Hyndman and Fan, 1996). For each current location Cell(i, j), the neighborhood can be expressed as:

$$126 \quad Nbh(i,j) = nbh(Cell(i,j), NW) \tag{2}$$

where *i* and *j* denote the row and column number of current cell at location (i, j), respectively;





- nbh(.) is the function for determining the neighborhood of Cell(i, j), and NW represents the
- 129 neighborhood window.
- 130 Then cells located within Nbh(i, j) form a cell set, which can be described as follows:

131 
$$CS_F(i,j) = \{Cell(i',j') \in \mathbf{R}_v \mid is\_in\_nbh(Cell(i',j'), Nbh(i,j)) == TRUE\}$$
(3)

where  $is_in_nbh(.)$  is the indicator function used to identify whether Cell(i', j') is located within the neighborhood Nbh(i, j); i' and j' are for the row and column number of the input value raster  $\mathbf{R}_v$ , respectively.

In Eq. (3), the detailed form of *is\_in\_nbh(.*) depends on the shape of the neighborhood
window. For example, when the window is circular, *is\_in\_nbh(.*) can be expressed as:

137 
$$\sqrt{(i'-i)^2 + (j'-j)^2} \le d$$
 (4)

where *d* is the radius of the circular window, i.e. window size, and *i* and *j*, and *i'* and *j'* are as explained above.

## 140 **2.1.3 Calculating the focal statistics**

Suppose that  $ST_F(Type, Set)$  denotes the statistical function of Focal Statistics, and Typeand *Set* are for the statistical parameter and the cell set to be processed. At the location of *Cell(i, j)* and under the Focal Statistics model, *Set* can be specified as  $CS_F(i, j)$ . Then the output of the Focal Statistics for *Cell(i, j)* can be expressed as:

145 
$$O_F(i,j) = ST_F(Type, CS_F(i,j))$$
(5)

147 
$$\mathbf{R}_{F out} = Focal\_Statistics(\mathbf{R}_{v}, NW, Type)$$
 (6)

where  $R_v$  and  $R_{F_{out}}$  represent the input value raster and the output raster for Focal Statistics, respectively, while *NW* and *Type* denote the functions for neighborhood window and statistical type in that order.

#### 151 2.2 Zonal Statistics model

152 Unlike Focal Statistics, which require only a value raster as input, Zonal Statistics require two





- 153 input raster layers: one as the value raster and the other as the zone raster. The zone raster
- 154 defines the shape and distribution of the zones, and each cell can only belong to a single zone.
- 155 Zonal Statistics calculates the statistics for each zone based on the corresponding cells from
- 156 the value raster, and the calculated statistic is assigned as the output value for all cells within
- 157 the zone. Finally, the output values of different zones are assembled into the output raster.
- 158 Zonal Statistics modeling involves two functional methods, which are for identifying the
- 159 cells in the value raster by zone and calculating zonal statistics respectively.

# 160 **2.2.1 Identifying cells in the value raster falling into each zone**

- 161 In Zonal Statistics, spatial overlay analysis can be used to find the zone code for each cell in
- 162 the value raster (Hyndman and Fan, 1996):

163 
$$Z_k(i',j') = Zone(Cell(i',j'))$$
(7)

where  $Z_k(i, j')$  represents the zone code at location (i, j'), and Zone(.) is the function that returns the zone code for the value raster cell at location (i, j').

For a given zone  $Z_k$ , the corresponding cells in the value raster form a cell set  $CS_Z(Z_k)$ , which can be expressed as:

168 
$$CS_{Z}(Z_{k}) = \{ Cell(i', j') \in \mathbf{R}_{v} \mid Zone(Cell(i', j')) = Z_{k} \}$$
(8)

#### 169 **2.2.2 Calculating the zonal statistics**

170 The calculation of statistics for a given zone  $Z_k$  can be represented as:

171 
$$O_Z(Z_k) = ST_Z(Type, CS_Z(Z_k))$$
(9)

- 172 It is important to note that the calculated statistics are assigned to all cells within each 173 zone, and the statistics for all zones are ultimately mosaicked into the output raster.
- 174 Using  $\mathbf{R}_v$  and  $\mathbf{R}_Z$  to denote the input layers of value raster and zone raster,
- 175 respectively. Zonal Statistics can be expressed as:

176 
$$\mathbf{R}_{Z_{out}} = Zonal_Statistics(\mathbf{R}_{v}, \mathbf{R}_{z}, Type)$$
 (10)

177 where  $\mathbf{R}_{Z_{out}}$  represents the output raster, and *Type* is for the statistic type.





## 178 2.3 Focal-Zonal Mixed Statistics

- 179 Similar to Zonal Statistics, Focal-Zonal Mixed Statistics also require two input raster layers,
- 180 and the specific modeling process involves the following two functional methods.

# 181 **2.3.1** Identifying cells within the neighborhood that belong to the same zone

Actually the determination of the target cell set in Focal-Zonal Mixed Statistics combines both the spatial proximity condition from Focal Statistics, and the environmental characteristic similarity condition from Zonal Statistics. For Cell(i, j) at the current location, if its neighborhood is Nbh(i, j) and its zone code is  $Z_k(i, j)$ , then its cell set consists of all cells within the neighborhood that belong to the same zone as the cell in Focal-Zonal Mixed Statistics. Mathematically, this can be expressed as:

188 
$$CS_{F-Z}(i,j) = \{Cell(i',j') \in \mathbf{R}_{v} \mid is\_in\_nbh(Cell(i',j'), Nbh(i,j)) == TRUE \\ Zone(Cell(i',j')) == Z_{k}(i,j) \}$$
(11)

## 189 2.3.2 Calculating the focal-zonal mixed statistics

190 Still using Type to represent the statistical type, the output result of Focal-Zonal Mixed

191 Statistics for the current Cell(i, j) can be expressed as:

192 
$$O_{F-Z}(i,j) = ST_{F-Z}(Type, CS_{F-Z}(i,j))$$
 (12)

194 
$$\mathbf{R}_{FZ out} = Focal_Zonal_Statistics(\mathbf{R}_v, \mathbf{R}_z, NW, Type)$$
 (13)

where  $R_v$ ,  $R_z$ , and  $R_{FZ_{out}}$  represent the value raster, zone raster, and output raster for Focal-Zonal Mixed Statistics, respectively; *NW* is the neighborhood window, and *Type* is

- 197 for statistical parameter.
- 198 **3 Module design**

## 199 3.1 Modeling process for Focal-Zonal Mixed Statistics

- 200 The flowchart for the newly proposed Focal-Zonal Mixed Statistics is presented in Fig. 1, and
- 201 the detailed modeling process is described as follows.







202

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

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

205 This initial step involves collecting and preprocessing the spatial data required for the analysis. The value raster typically represents the primary variable of interest, i.e., the target 206 207 layer, such as temperature, pollution levels, or vegetation indices. Environmental factor 208 rasters include various influencing factors, such as elevation, slope, land cover, and other 209 relevant geographical features that may contribute to the heterogeneous distribution of the 210 target layer. Preprocessing methods may include resampling, reprojecting, and normalizing 211 the data to ensure consistency and compatibility among the raster layers, so that they share the 212 same spatial extent, resolution, and reference system.

213 (2) Construction of unique-value environmental characteristic zonal raster (UV-ECZR)

This process can be achieved using the "Reclassify" tool in ArcGIS 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 unique-value encoding. Cells in the UV-ECZR that share the same unique-value





- 218 environmental characteristic code (UV-ECC) form a similar environmental unit (SEU). A
- 219 detailed implementation of this process is described in the following Sect. 3.2.1.
- 220 (3) Determination of neighborhood window and statistical parameters
- 221 This process involves defining the neighborhood window and specifying the statistical
- 222 parameters for Focal-Zonal Mixed Statistics.
- 223 (4) Preparation of output raster
- This step involves creating an output raster with the same spatial extent, resolution, and reference system as the input rasters. This output raster will store the results of the
- 226 Focal-Zonal Mixed Statistics calculations.
- 227 (5) Calculation of the statistics
- In this step, the moving window technique is applied to locate each current cell and its local window. For each current cell, identify the neighborhood cells based on the defined neighborhood window parameters (refer to Sect. 2.1.1). Within this neighborhood, isolate the cells within the same SEU as the current cell. Subsequently, calculate the specified statistic for these cells in the value raster that correspond to those isolated cells.
- 233 (6) Save of output raster
- 234 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.
- 237 **3.2** Core algorithm design for Focal-Zonal Mixed Statistics
- 238 3.2.1 Algorithm design for the UV-ECZR construction
- Assume that there are p continuous environmental variables, i.e.,  $E_1, E_2, \ldots, E_p$ , with their
- 240 corresponding reclassified variables being  $CE_1, CE_2, \dots, CE_p$ . The number of categories and
- 241 the digit lengths of these categories are denoted as  $S_1, S_2, \ldots, S_p$  and  $D_1, D_2, \ldots, D_p$ ,
- respectively. The method for calculating the digit lengths of the categories is as follows:





243 
$$D_q = \lfloor \lg S_q \rfloor + 1$$
 (14)  
244 where  $\lg$  denotes the logarithm with base 10,  $\lfloor . \rfloor$  represents the floor function, and  $q =$   
245  $1, 2, ..., p$ . The categories for the  $q$ -th environmental variable should be a positive integer,  
246 and the range of cell value in the reclassified raster ( $CE_q$ ) can be expressed as  $\lfloor 1, S_q \rfloor$ .  
247 Then, the UV-ECC at location  $(i, j)$  can be defined as:  
248  $UV - ECC$   $(i, j) = 1 \xrightarrow{D_1} D_2 \dots D_q \dots D_p$   
249 where  $\overline{X \cdots X}$  represents the category code of  $CE_q$  at location  $(i, j)$ ,  $D_q$  is obtained through  
250 Eq. (14). To keep the consistency in the UV-ECC format, it is necessary to prepend a  
251 sufficient number of "0"s to ensure the digit length of category code equals  $D_q$ .  
252 In the form of raster calculator, the UV-ECZ R can be expressed as:  
253  $UV - ECZR = CE_1 \cup CE_2 \cup ... \cup CE_p$  (16)  
254 where U represents the spatial overlay.  
255 **3.2.2 Algorithm design for determining the valid range for statistics under the sliding**  
256 window technique  
257 A rectangular window, which aligns with the rows and columns of raster data and is both easy  
258 and efficient to implement, is commonly used in the sliding window technique. However, its  
259 drawback is also evident: the grid cells at the four corners are much farther from the current  
250 location than those on the horizontal and vertical axes (Zhang et al., 2016a). Despite this,  
259 rectangular windows remain one of the most popular forms of spatial sliding windows. In this  
250 study, we consider rectangular windows along with circular and elliptical windows. Since a  
251 circle is a special form of an ellipse, we use the ellipse as an example to illustrate the  
252 algorithm design for determining the valid range for statistics under the sliding windows  
253 technique in Focal-Zonal Mixed Statistics.

266 (1) Mask matrix for elliptical window





267 An elliptical window is defined by three key parameters: the length of major axis, the 268 ratio of the minor axis to the major axis, and the deflection angle of major axis. Let  $(x_0, y_0)$ 269 represent the center of the ellipse, i.e., the current location, *a* denotes the semi-major axis 270 length, *r* be the minor-to-major axis ratio, and  $\theta$  be the deflection angle. Then the elliptical 271 window can be mathematically expressed as:

272 
$$Ellipse((x_0, y_0), a, r, \theta) = \frac{[(x - x_0)\cos\theta + (y - y_0)\sin\theta]^2}{a^2} + \frac{[-(x - x_0)\sin\theta + (y - y_0)\cos\theta]^2}{(ra)^2}$$
(17)

Based on Eq. (15), the bounding box of the elliptical window can be represented as *BBox<sub>ellipse</sub>(minX, maxX, minY, maxY)*, where *minX, maxX, minY, maxY* are as follows:

275 
$$\begin{cases} minX, maxX = x_0 \pm \sqrt{\frac{4CF}{B^2 - 4AC}} \\ minY, maxY = y_0 \pm \sqrt{\frac{4AF}{B^2 - 4AC}} \end{cases}$$
(18)

276 here,

277 
$$\begin{cases}
A = a^{2} (\sin^{2} \theta + r^{2} \cos^{2} \theta) \\
B = 2a^{2} (r^{2} - 1) \sin \theta \cos \theta \\
C = a^{2} (\cos^{2} \theta + r^{2} \sin^{2} \theta) \\
F = -\frac{1}{2} (Dx_{0} + Ey_{0}) - r^{2} a^{4}
\end{cases}$$
(19)

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 mask is used directly to define the area of interest for statistics, see Fig. 2a.

283









Figure 2. 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

288 (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<sub>Similarity\_mask</sub>* to represent this unit, cells with





the same environmental characteristic code as the current cell are assigned a value of "True", 293 while others are assigned a value of "False", as shown in Fig. 2b. 294 295 (3) Mask matrix for similar environment in the elliptical window 296 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 297 298 a logical "AND" operation between these two matrices, as expressed in the following 299 equation: 300  $Matrix_{E_s_{mask}} = Matrix_{Similarity_{mask}} \land Matrix_{Ellipse_{mask}}$ (20)where  $\wedge$  denotes the logical "AND" operator. Matrix<sub>E S mask</sub> serves as the basis for 301 302 determining the valid range for Focal-Zonal Mixed Statistics, as illustrated in Fig. 2c. 3.2.3 Algorithm design for the statistics calculation 303 304 The algorithm for the statistics calculation is designed as follows: 305 (1) Determination of valid statistical cells in the value raster 306 Using Matrix<sub>Value</sub> to represent the cell array from the value raster within the bounding box defined above, then by performing a bitwise multiplication of  $Matrix_{ESmask}$  with 307  $Matrix_{Value}$ , the final valid statistical value matrix  $Matrix_{Valid}$  is obtained: 308  $Matrix_{Valid} = Matrix_{E \ S \ mask} \otimes Matrix_{Value}$ (21)309 where & denotes bitwise multiplication. This operation collects cells from the value raster that 310 are located within the neighborhood and share the same UV-ECC as the current cell, while 311 masking out other cells that could interfere with the statistical results. In Matrix<sub>Valid</sub>, the 312 313 masked cells can be represented with "NaN". (2) Design of the calculation function for the statistics 314 Taking Matrix<sub>Valid</sub> as the final input, the calculation functions for Focal-Zonal Mixed 315 Statistics can be designed based on scientific computing tools such as NumPy. This library 316 provides a range of statistical methods, including minimum, maximum, mean, standard 317





| 318 | deviation, percentiles, and more. For instance, the "numpy.nanmax()" method can ignore          |
|-----|---|
| 319 | "NaN" values and return the maximum value of $Matrix_{Valid}$ , while the                       |
| 320 | "numpy.nanpercentile()" method, also ignoring "NaN" values, calculates the n-th percentile      |
| 321 | of Matrix <sub>Valid</sub> .  |
| 322 | 3.3 User interface design   |
| 323 | The Focal-Zonal Mixed Statistics, along with traditional Zonal Statistics and Focal Statistics, |
| 324 | are included in the newly developed toolbox, FZStats v1.0, using Python3 and QT5. The user      |
| 325 | interface is organized into three tabs, each dedicated to one of the three methods, allowing    |
| 326 | users to switch among them (see Fig. 3). Taking the tab for Focal-Zonal Mixed Statistics as an  |
| 327 | example, the interface is divided into four main sections, and the detailed description of the  |
| 328 | user interface design is given as follows.  |
| 329 | (1) Input and output design   |
| 330 | Users can select the value raster and UV-ECZR as input data from their datasets.                |
| 331 | Additionally, they can specify the output path and filename for the resulting raster data.      |
| 332 | (2) Neighborhood window design  |
| 333 | Users can configure the shape (e.g., rectangular, circular, elliptical) and size (e.g.,         |
| 334 | number of cells or spatial units) of the neighborhood window. For rectangular and circular      |
| 335 | windows, size is specified by the half-side length and radius, respectively. Elliptical windows |
| 336 | are characterized using three morphological parameters: the length of the major axis, the ratio |
| 337 | of the minor axis to the major axis, and the deflection angle of major axis.                    |
| 338 | (3) Statistical measure design  |
|     |   |

Users can select a specified statistical measure from the dropdown menu. For percentile
calculations, users are required to specify the exact percentile values of interest, such as the
50th, 75th, or 98th percentiles.

342 (4) Optimization settings

15





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

Chunk processing: Users can divide the input raster into smaller chunks, which can enhance performance by reducing the memory load and making it easier to handle large datasets.

Parallel processing: Users can configure the number of processors used for 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.

Threshold setting: Users can specify 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 results.

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

16





| Yocal Stats Zo  | nal Stats FZ Mixed Stats  |                               |      |   |
|---|---|-------------------------------|------|---|
| Rasters Setting   |   |                               |      |   |
| Value Raster  | E:/rn/3_works/CBS/LST/LST_STD   | ).tif                         |      |   |
| Zone Raster   | E:/rn/3_works/CBS/HJTZ/AS/AS_   | _class. tif                   |      | 2 |
| Result Raster   | E:/rn/3_works/CBS/AS/as_rst/o   | vir240_mean_fz.tif            |      |   |
| Neighbourhood S   | etting  | Statistics Setting            |      |   |
| Window Type   | CIRCLE ~  | Statistics Type               | MEAN | ~ |
| Radius  | 240   |                               |      |   |
|   |   | Advanced Setting              |      |   |
|   |   | Sub-gridding                  | 1, 1 |   |
| Units   | 🗿 Cell 🔵 Map  | Process Number                | 16   |   |
|   |   | Threshold                     | 1    |   |
|   |   | 🛃 Ignore Nodata               |      |   |
| Processing Mess   | age   |                               |      |   |
| Value Raster: E:<br>Zone Raster: E:/<br>Result Raster: E:/<br>Unit: Cell<br>Neighbourhood Wi<br>Radius: 240<br>Statistics Type:<br>Columns: 1<br>Rows: 1<br>Process Number: | /rn/3_works/CBS/LST/LST_STD.ti<br>rn/3_works/CBS/HJTZ/AS/AS_clas<br>:/rn/3_works/CBS/AS/as_rst/cir?<br>ndow: CIRCLE<br>MEAN<br>16 | f<br>s.tif<br>240_mean_fz.tif |      |   |

361

362 Figure 3. User interface design of FZStats v1.0

# 363 4 Experimental study

# 364 **4.1 Background of the case**

Geothermal, like coal, oil, and natural gas, is a valuable energy mineral resource, and its development and utilization play a significant role in alleviating energy supply pressure and improving the global environment (Huang and Liu, 2010; Goldstein et al., 2011). The most important indicator for geothermal resource exploration is thermal anomalies (Romaguera et al., 2018; Gemitzi et al., 2021). In recent years, with the rapid development of remote sensing, Land Surface Temperature (LST) derived from thermal infrared bands has become a key





method for identifying geothermal anomalies. However, LST is influenced by various factors,
including not only geothermal activity but also 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 caused by geothermal activity, it is necessary to suppress the influence 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 abnormal information from geothermal activity.

## 380 **4.2 Data preprocessing**

## 381 4.2.1 Spatial distribution of LST

Landsat 8 images (Orbit Number: 116031) observed on September 16, 2013 covering the 382 study area, i.e., Changbai Mountain region, were used for LST mapping and geothermal 383 exploration in this study. After preprocessing operations such as radiometric calibration and 384 385 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 386 Fig. 4. By comparing Figs. 4 and 5, it can be seen that there is a strong spatial correlation 387 388 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 389 LST exhibited significantly higher values on the southeast-facing slopes than on the 390 391 northwest-facing slopes.







392

393 Figure 4. Spatial distribution of land surface temperature (LST) in the study area

## **4.2.2 Mapping of unique-value environmental characteristic zones**

395 The slope and aspect were used as environmental factors to construct the UV-ECZR (Fig. 5a and b). As previously mentioned, these two factors have a strong spatial coupling relationship 396 397 with LST. Although elevation and vegetation coverage were not directly applied in environmental zoning, they can be considered similar within the neighborhood window 398 399 (Zhang et al., 2019). Therefore, their effects are indirectly suppressed. In other words, in Focal-Zonal Mixed Statistics modeling, sample heterogeneity caused by long-range spatial 400 variables can be controlled through spatial proximity, while that brought by short-range 401 402 spatial variables can be suppressed through environmental similarity.







403

404 Figure 5. Maps of environmental factors: (a) slope aspect, (b) Slope degree, and (c) the composite
405 unique-value environmental characteristic zonal raster (UV-ECZR).

# 406 4.3 Enhancement of geothermal anomalies based on Focal-Zonal Mixed Statistics

In mineral prospectivity mapping, standard deviation standardization is often employed to assist in constructing indicator variables for prospecting. This process 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 value deviates from the mean. The essence of this method lies in determining the appropriate range for calculating the mean and standard deviation, enabling a comparison of the current value against the mean and using





the standard deviation to quantify this difference. In this study, Focal-Zonal Mixed Statistics 413 414 was used for this purpose, i.e., defining the comparable sample range based on both spatial proximity and environmental similarity. Specifically, in this case, the level of LST at each 415 416 current location is assessed within the range determined by both the local window and the 417 similar terrain features. This approach mitigates the influence of factors such as terrain and 418 vegetation, thereby producing a distribution map of LST anomalies that predominantly reflects geothermal activity. When the current window is a circle with a radius of 7.2 km, the 419 final enhanced geothermal anomaly is shown in Fig. 6. 420



421

422 Figure 6. Enhanced geothermal anomaly map based on Focal-Zonal Mixed Statistics with a local window

<sup>423</sup> radius of 7.2 km.





- Comparing Figs. 5 and 6, it is evident that the LST anomalies enhanced using Focal-Zonal Mixed Statistics exhibit a better spatial correlation with known geothermal wells (obtained from Yan et al., 2017), and their high values indicate known geothermal wells more effectively. Therefore, we have reason to believe that the high-value areas in Fig. 6 have a higher probability of revealing new geothermal resources.
- 429 **5 Discussion**

## 430 5.1 Advantages of the new statistics

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.





448



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.

#### 454 **5.2 Robustness of the new method**

To ensure that the superior performance of the new model in Sect. 5.1 is not coincidental, it is necessary to adjust parameters such as the local window size and the geothermal well representative area and conduct multi-scenario comparison experiments. This will help analyze the robustness of the new model's advantages.

When the representative area for a geothermal well is determined by 0.1km, 0.2km, and 0.3km buffers, respectively, the AUC values for LST and its enhancement indices are calculated. These values, obtained through different models under various local window radii, are plotted on a Cartesian coordinate system, as shown in Fig. 8.







Figure 8. The changes in AUC values with the window size of Land Surface Temperature (LST) and its three enhancement indicators obtained by Focal Statistics, Zonal Statistics, and Focal-Zonal Mixed Statistics, when a geothermal well represents circles with a radius of (a) 0.1km, (b) 0.2km, and (c) 0.3km, respectively.

Overall, the two enhancement models incorporating neighborhood windows, i.e., Focal 468 Statistics and Focal-Zonal Mixed Statistics, perform better than the Zonal Statistics model and 469 470 the LST without enhancement. The poor performance of Zonal Statistics is due to the strong spatial variability of LST and the simplicity of the classification scheme used. Additionally, 471 since local window methods are sensitive to spatial scale, the performance of Focal Statistics 472 473 and Focal-Zonal Mixed Statistics varies with the window size. However, regardless of whether the geothermal well representative area is 0.1km, 0.2km, or 0.3km, the performance 474 of Focal-Zonal Mixed Statistics consistently surpasses that of Focal Statistics. 475

## 476 5.3 Advancements of the Toolbox

The FZStats v1.0 developed in this study not only integrates traditional Focal Statistics and Zonal Statistics, which deal with SPD and SSH respectively, but also innovatively implements Focal-Zonal Mixed Statistics based on spatial proximity and environmental similarity, addressing both SPD and SSH. Therefore, this toolbox is expected to provide a novel solution to spatial statistics.





A variety of parameter setting interfaces are provided to enhance the statistical 482 applicability of the developed toolbox, ensuring it meets the requirements of different 483 application scenarios and computing conditions. In terms of neighborhood window settings, 484 485 in addition to rectangular and circular windows, an elliptical window is also available, allowing users to express spatial anisotropy in the neighborhood through elliptical parameters. 486 487 Regarding statistical parameters, the new toolbox supports traditional metrics like mean, standard deviation, minimum, and maximum values, as well as calculations for arbitrary 488 percentiles. To make the best use of memory and CPU capabilities, the toolbox supports raster 489 490 data chunk processing and multi-process modes, accommodating different computer memory capacities and enabling parallel processing on multi-core CPUs. Additionally, users can set a 491 minimum cell number of samples for statistics through the "Threshold" parameter to avoid 492 493 low statistical precision and unreliable results due to insufficient sample size.

Lastly, to enhance automation and efficiency in multitasking, the toolbox provides a batch processing solution. Users can write parameters into an INI-format multi-section configuration file, which avoids repetitive and tedious manual operations. This can not only enable one-time setup and automatic execution of multiple tasks, but support parameter reuse and error tracing.

## 499 6 Conclusions

This study developed the FZStats v1.0 toolbox using Python3 and QT5. The new toolbox integrates Focal Statistics, Zonal Statistics, and the newly developed Focal-Zonal Mixed Statistics. We provided detailed algorithm implementations and modeling processes for these methods and evaluated their performance in geothermal anomaly identification. The main conclusions are as follows: First, the development of the Focal-Zonal Mixed Statistics is essential, as it addresses gaps that traditional Focal Statistics and Zonal Statistics cannot fill. Second, FZStats v1.0 offers extensive parameter setting options, supporting different window





- 507 shapes and types of statistics; simultaneously, by adjusting processing parameters, it can 508 ensure efficient performance on computers with varying configurations. Third, case analyses 509 show that Focal-Zonal Mixed Statistics significantly enhance geothermal anomalies compared 510 to Zonal Statistics and Focal Statistics methods, with this advantage being robust.
- In summary, FZStats v1.0 not only innovates spatial statistical methods theoretically but also demonstrates powerful functionality and flexibility in practical applications, making it a promising tool in the field of geothermal anomaly identification and other areas requiring spatial statistical solutions.

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- 519 *Code availability.* The source code for FZStats v1.0 is available on GitHub at 520 https://github.com/Renna11/FocalZonalStatistics. The latest version of the software can be 521 obtained at https://zenodo.org/records/13208114.
- Data availability. The sources of the original data supporting the case study in this paper are 522 as follows: (1) Landsat 8 images used in this research were downloaded from 523 524 https://earthexplorer.usgs.gov (last accessed: 3 August 2024); (2) Land Surface Temperature data can be obtained from http://databank.casearth.cn (last accessed: 3 August 2024); (3) 525 original elevation data used for calculating slope and aspect is from the Shuttle Radar 526 Topography Mission (SRTM) Global 1 Arc-Second Product, provided by NASA, available at 527 https://earthexplorer.usgs.gov (last accessed: 3 August 2024); and (4) geothermal well data is 528 sourced from Yan al. (2017).Sample data be found 529 et can at https://zenodo.org/records/13766015. Readers can refer to the instructions provided in the 530 531 "README.md" file on the code repository (https://github.com/Renna11/FocalZonalStatistics)





- 532 for guidance on software use, which allows for the reproduction of the case analysis using the
- 533 aforementioned original data.
- 534 Author contributions. DZ and QC conceived the original idea. NR and DZ developed the
- 535 software. NR handled data processing and drafted the manuscript. DZ and QC revised the
- 536 manuscript. All authors read and approved the final manuscript.
- 537 *Competing interests.* The authors declare no competing interests.
- 538

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