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### A gradient model for the spatial patterns of cities

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#### 1 Abstract

The dynamics of city's structures are determined by the coupling of functional 2 3 components (such as restaurants) and human population. Yet, there still lacks mechanism models to quantify the forces on spatial distribution of the components. Here, a gradient 4 model is explored to simulate the individual density curves of multiple types of city 5 functional components based on the equilibria of gravitational and repulsive forces along 6 7 the urban-rural gradient. The model is concise for it relying four key variables, the attributes of components include net ecosystem service (m) and environmental index  $(\gamma)$ , 8 9 and the attributes of cities include land rent exponent ( $\sigma$ ) and population attenuation 10 coefficient ( $\beta$ ). The model has been used to simulate the distribution curves of 22 types of 11 components on the urban-rural gradients in 13 cities in two periods. The model reveals a bottom-up mechanism that the patterns of the components in a city are determined by the 12 13 economic, ecological, and social attributes of both cities and components. Strongly 14 backed by empirical data, our model can predict the distribution curves of many types of 15 components along with the development of cities. This model provides a general tool for 16 analyzing the distribution of multiple objects on the gradients.

17

18 Keywords: environmental index, population pattern, urban-rural gradient, land rent,
19 transport costs.

#### 1 Main Text

#### 2 Introduction

3 A fascinating event in human activities is the formation, development, expansion, and renewal of cities (1-3). A city is composed of human beings and multiple types of 4 functional components (or namely facilities), which are enterprises, firms, and other 5 6 institutions that provide goods and services for people (4, 5). The enclosed industrial components are just defined as organaras (big organs) considering a modern industrial 7 city as a super-cell living system and a city center is a citynucleus (6). Some types of 8 9 components, such as banks and restaurants, are concentrated near citynucleus (7). In contrast, as a city develops, some components, such as manufactories, tend to move 10 outward from the city center (8, 9), while some emerging industries (such as delivery 11 stores) spring up in the urban area (Fig. 1a). The emergence, coexistence, competition, 12 migration, and extinction of the components shape the spatial structure of the city (9-11). 13 14 The studies on city structure are limit in theoretical derivation and left many crucial 15 questions. For example, how much is the impact of land rent on the distribution of 16 functional components? How the population pattern drives the change of component 17 spatial distribution? How the residents' ecological preferences drive the change of 18 component distribution? To uncover the evolutionary mechanism of the components on 19 the gradients can deepen the fundamentally understood of city's functional spatial 20 structure.

In general, each type of functional component has many individuals in a city (5, 12, 13). For example, a type of fast food restaurant can be seen as a group and occupies a niche in a city, a phenomenon akin to a biological population within a community (14).

The present models for the number of components are statistical and they study the 1 response of the local individual density of components—for example, the number of 2 3 restaurants, schools, hospitals, and banks—to the human population density in a location (15-17). These models can explain neither the whole city's structure nor the complex 4 driving forces—apart from the population—behind the distribution of components. A 5 series of spatial economic models, pioneered by von Thünen, can explain the mechanism 6 for the locations of land use types and functional components that affected by land rent 7 and transport cost gradients (3, 18, 19-21). However, these spatial economic models have 8 9 not involved the impact of people's ecological preferences. This study adopts the physics methodology while referring to the relevant theories of geography and tries to uncover 10 11 the mechanism of city structure and the evolution.

12

#### 13 The spatial pattern of city components in urban-rural landscapes

14 In this paper, a 'city' means an urban-rural system, which has been defined as a 15 eukarcity (6). A great number of various types of functional components separate or 16 overlapping distribute in city core (citynucleus) and the periphery rural areas (Fig. 1a). 17 We investigate 24 types of components and choose 4 types that implement urban processes that meet the living demands of the local residents. The real-world data of two 18 19 years of the components are investigated and compiled. Results showed that the 20 Kentucky Fried Chicken shops (KFC) are concentrated near the citynucleus (Fig. 1b), the Zhongtong express outlets (ZTO), which provides domestic parcel service, are 21 concentrated on the outer side of KFCs; the cultivated greenhouses (GHs) are located in 22 23 suburban areas near the urban fringe, and the dairy farms (DF) are located in ex-urban

areas. Each type of component has  $\sim 10^2$  to  $\sim 10^3$  individuals in a city except for dairy 1 farms, which are rare (SI Appendix, Table S1). The individual density of a type of 2 3 component varied with the distance (d) from the citynucleus (Fig. 1c). The univariate polynomial regressions show that, for a type of component, the individual density curve 4 has a peak  $(P_{max})$ , which is located at a position  $(d^*)$  along the urban-rural gradient (Fig. 5 6 1c and SI Appendix, Table S2). The rank correlation showed that the  $d^*$  of a type of component is related to the supply ability of the target services, which is the economic 7 return to the investor for constructing and operating the components (Fig. 1c, d). An 8 9 exception is that the  $d^*$  of DF is outside GH although the net service, which is the sum of target and accompanied services, of DF is higher than GH. We find that the higher  $\gamma$ 10 11 value, which is the ratio of environmental impacts to target services, pushes DF outside GH (*SI Appendix*, Table S2), and we denote  $\gamma$  as the 'environmental index'. The statistical 12 13 model (22) we used can help us acquire the characteristics of component distribution (SI 14 Appendix, Table S2), but cannot uncover the driving factors and mechanisms.

15

#### 16 Modeling overview

The distribution patterns of the functional components are mainly driven by economic factors (19, 23). The components, which are artificial systems, need to provide enough economic returns (target services) to the investors. The economic constraints for the distribution of components are the land rent and transport costs (23), while the ecological constraints are environmental impacts (8). In an ideal city with no geographical difference (19) and only one citynucleus, the human population density monotonically decreases from the urban center to rural areas, within which the components are located and provide services for people (Fig. 2a). The two-dimensional pattern of attributes of city and components can be described as a one-dimensional individual density curve along the urban-rural gradient, P(d), in a city (Fig. 2b, c). It is emphasized that, although the above principle depicts a single-center city, it also suitable for polycentric cities. The gradient and equilibrium of gravitational and repulsive forces can also be separated from the sub-center of a polycentric city.

7 The gravitational force  $(F_g)$  along an urban-rural gradient for a type of component is mainly determined by the spatial pattern of the product's transport cost. For the life-8 9 support components (such as restaurants), the cost of the products of a component is negatively correlated to the density of local human population (Fig. 2d). The 10 11 transportation cost depends on human population density, road condition, and product transportability (19, 24). Densely populated areas attract the distribution of functional 12 13 components (15, 25) due to a small average transportation distance  $(\bar{r})$  from products to 14 consumers (*SI Appendix*, Fig. S9a). In the citynucleus, the population is much higher than in urban fringe and rural areas (19, 24). For the human population density in locations in 15 response to the distance (d) from citynucleus, the exponent function  $(Y = ae^{bX})$  is best fit 16 17 that support Clark (26) if the range limit to urban areas; while if include the suburban area, the power law function is the best fit regressions (SI Appendix, Table S8), 18

19

$$Pop(d) = Ad^{\beta} \tag{1}$$

where Pop(d) is the average human population density of the ring located at distance *d* from the citynucleus. The Pop(d) values were measured through random quadrat investigation on the ring (Fig. 2a). *A* is the fitted coefficient. The attenuation coefficient ( $\beta$ ) is for the human population density on the urban-rural gradient. 1 Based on the negative correlation between product transportation distance and 2 population density (23), the mean distance  $\bar{r}$  for a type of component at *d* ring is,

$$\bar{r}(d) = -\beta \ln\left(d\right) \tag{2}$$

where r̄(d) is the average 'last kilometer' distance between the components' products
and the consumers at location d on the urban-rural gradient, d and β are come from
equation (1).

The transport cost also depends on product transportability, which varied greatly 7 among different types of components. For example, we have found that the transport of 8 9 KFC's take-out products is limited to 3 km in the case cities according to the distribution 10 rules of stores. With the development of the urban and peri-urban agriculture, the vegetables from the greenhouse can be transported more than 30 km and keep fresh for 11 local acceptance (SI Appendix, Fig. S9b). The 'iceberg transport model' to calculate the 12 value loss in the transportation process (27) is introduced to calculate transport cost ( $C_T$ ) 13 of the products, 14

15

3

$$C_T(d) = I (1 - e^{-\tau \bar{r}})$$
 (3)

16 where  $C_T(d)$  is the transport cost at location d on the urban-rural gradient, I is the 17 coefficient for the initial value of a type of product;  $\tau \in (0,1)$  is the iceberg coefficient, 18 which is the proportion of value lost per unit of distance transported.

#### 19 Combining equations (2) and (3),

20 
$$F_g(d) = I(1 - e^{\tau \beta \ln(d)}) = I(1 - d^{\tau \beta})$$
 (4)

where  $F_g(d)$  is the gravitational force on urban-rural gradient in a city. Equation (4) shows that the attraction is monotonic decreasing from citynucleus to rural area (Fig. 2d). 1 The repulsive force  $(F_r)$  along an urban-rural gradient is monotonic decreasing from 2 citynucleus outward. Generally, the high land rent (LR) repulses some low economic 3 output components away from the city center (19, 28). Only the components with high 4 economic output can be located near the citynucleus as they can afford paying the high 5 land rent. We have found that the land rents (LR) in most cities were power law 6 decreasing on the urban-rural gradient (18),

7

13

$$LR(d) = cd^{\sigma} \tag{5}$$

8 where LR(d) is the land rents at location d on the urban-rural gradient, c is the land rent 9 coefficient (USD m<sup>-2</sup> yr<sup>-1</sup>), and  $\sigma$  is the land rent attenuation coefficient.

Besides the impact of land rent, a functional component's economic outputs (m) and people's preference for environmental impacts also affect the  $F_r$  for a type of component, i.e.,

$$F_r(d) = LR(d) / (m/\gamma) = cd^{\sigma} / (m/\gamma)$$
(6)

14 where  $F_r(d)$  is the repulsive force at location d on the urban-rural gradient,  $\gamma$  is the 15 absolute value, m > 0. Equation (6) means that a larger net ecosystem service enables a 16 component to be distributed near the citynucleus, while a larger ecosystem dis-service 17 pushes the component outwards (*SI Appendix*, Fig. S9c). For example, with the social 18 prosperity in recent decades, the components with high environment impacts are moved 19 far from the citynucleus due to people's growing preference for better environmental 20 quality.

The minimum of gravitational plus repulsive forces  $(F_g + F_r)$ , *E*, is changing with the development of city, and it is also different among different types of components in a city (Fig. 2d). The optimum location (*d*\*) corresponds to the *E* for a type of component on the urban-rural gradient where the maximum individual density (*P<sub>max</sub>*) occurs (Fig. 2b,
c). Each type of component has a *d*\* and some of them can overlap due to fact that they
are distributed across different locations within a ring (Fig. 2a).

The total amount of a type of component and the  $P_{max}$  in a city is determined by the total demand (*M*) and the net ecosystem service (*m*) of the component. We follow the form of Newton's gravity model and take the product of these two terms ( $M \times m$ ) as the numerator term. Then the individual density of a type of component along an urban-rural gradient is

$$P(d) = G \frac{M \times m}{Fg(d) + Fr(d)}$$
(7)

10 where P(d) is the component density t location d on the urban-rural gradient, G is a 11 coefficient to adjust the order of magnitude of the  $M \times m$  multiplier.

12 When equations (4) and (6) are substituted into equation (7), we get that the 13 individual density curve of a type of component on the urban-rural gradient is

14 
$$P(d) = G \frac{M \times m}{I(1 - d^{\tau\beta}) + cd^{\sigma}/(\frac{m}{\gamma})}$$
(8)

15 The constant of proportionality (G) in equation (8) will be acquired via the16 simulation of the real-world data.

17

#### 18 Model optimization

19 The input variables were calculated using the above equations and then simulate the 20 individual density curves using equation (8). The model fitting is based on the 21 Levenberg-Marquardt algorithm, which can provide numerical solutions of nonlinear 22 minimization (local minimum). The parameters and coefficients (*SI Appendix*, Table S3,

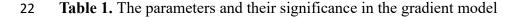
Tables S5,6,9) were input to the nonlinear fitting module (using Origin Pro 2018, 1 OriginLab Corporation) to estimate the coefficients (G, I) by fitting the real-world data of 2 3 the 4 types of functional components in 13 cities. The fitting accuracy of the model parameters is evaluated and improved in iteration and this process continues until the 4 accuracy of the model parameters can no longer be improved. Unfortunately, the 5 simulated distribution individual density curves of KFC, ZTO and GH on the urban-rural 6 gradient in most cities were not good fits to the data, and particularly, the kurtosis did not 7 conform to the real-world data. This means that equation (8) overlooks some factors. 8

9 After re-evaluation, a new parameter, *Z*, was introduced into the denominator of the 10 model. Finally, we finish the construction of a gradient model for functional components 11 along urban-rural gradients,

12 
$$P(d) = G \frac{M \times m}{I(1 - d^{\tau\beta}) + cd^{\sigma}/(\frac{m}{\gamma}) + Z}$$
(9)

where parameter Z represents the other factors besides the gravitational and repulsive forces in the model and we dubbed Z as the 'city index' due to it being related to the city attributes revealed by statistics. We did not further simplify the mathematical form of equation (9) because each parameter has physical significance and corresponds to the mechanism behind the distribution of components.

All the meanings of the model parameters are shown in Table 1. After validating the simulation of distribution of multiple types of components, the gradient model (eq 9) was used to predict the patterns of components in different periods or different cities.



Parameters	Symbol
Input variable	
Total demand for specific goods and services of cities	M
Net ecosystem services of the components	т
Iceberg attenuation index in transportation of products	τ
Coefficient of statistical function of population distribution	β
Distance from citynucleus	d
Coefficient of statistical function of land rent distribution	С
Land rent attenuation power	σ
Ratio of ecosystem dis-services to target services	γ
Simulated or adjusted parameter	
Adjustment constant for $M \times m$	G
Coefficient in transport cost function	Ι
City index	Ζ

#### 1

#### 2 **Results**

#### **3** Model simulation and validation

Using the model (eq 9), we run the fitting module again. The simulated individual 4 density curves coincide with the real-world data in two periods (Fig. 3a-d and SI 5 Appendix, Table S3). Results showed that the fittings are significant (the minimum  $R^2 >$ 6 7 0.72 of the fitting curves). The individual density curves and the relationships between the gravitational and repulsive forces support our hypothesis in Fig. 2. The simulation for 8 the individual density curves of the components shows that the repulsive forces to the 9 four components are ordered KFC < ZTO < GH < DF, and so are the gravitational forces 10 11 (Fig. 3e-h). The minimum points (E) of repulsive plus gravitational forces correspond to the  $d^*$  (SI Appendix, Table S2). For example, along with the development of Shanghai 12

City, the curve of land price and population along the urban-rural gradients tend to be 1 gentle (absolute values of  $\sigma$  and  $\beta$  decrease), resulting in the  $P_{max}$  of KFC, ZTO, GH and 2 3 DF decreasing by 20%, 29%, 13%, and 21% respectively, and all the  $d^*$  moving outwards (Fig. 3a-d). The reason is that with the development of the city, both gravitational and 4 repulsive forces for the four components increase and the equilibrium changes (Fig. 3e-5 h). All the above model behaviors support our hypothesis in Fig. 2, which is that the 6 equilibrium of forces determines the  $d^*$ , and the city's attributes determine  $P_{max}$ . In 7 addition, the  $d^*$  of GH is located at the edge of the built-up area, which reflects the shape 8 9 and size of the urban area (Fig. 3c). This means that the driving force of the components quantified by the gradient model can be used to study the evolution of the scale of cities. 10

11 The 4 types of components simulated by the gradient model in 13 cities showed that all the individual density curves of the components fitted the real-world data significantly 12 except for KFC in Shaoxing City and ZTO in Jiaxing City, where there are insufficient 13 14 individuals for simulation (Fig. 3-4 and SI Appendix, Fig. S1). The individual density curves of KFC, ZTO, GH and DF were simulated well by gradient (P < 0.05), with 15 average R<sup>2</sup> of 0.88, 0.81, 0.77, and 0.87, respectively. More importantly, the gradient 16 17 model can simulate the individual density curves of multiple components (based on 18 corresponding coefficients and parameters) in a city at the same time, and simulate their 19 coexistence at any location within cities (Fig. 4 and SI Appendix, Fig. S2). The gradient 20 model clearly shows the mechanism of gravitational-repulsive force shapes the specific niche of components on the urban-rural gradient (SI Appendix, Fig. S3). 21

22

#### 23 Prediction and application ability of the gradient model

In order to validate the robustness and the predictive power of the gradient model, 1 we analyze the relationships between the coefficients of the model and the attributes of 2 3 the case cities and components. Regression analysis shows that the Z of the components which are located in urban areas are related to urban central land price (c), while the Z of 4 components which are located in rural areas are most closely related to urban areas (SI 5 Appendix, Fig. S4). However, I is not related to any attributes. We then try to find if there 6 are indirect relationships, and then the aggregate force of the model, the gravitational and 7 repulsive forces is derived, 8

9 
$$F'(d^*) = \left[ I \left( 1 - d^{*\tau\beta} \right) + c d^{*\sigma} / \left( \frac{m}{\gamma} \right) \right]' = 0$$
 (10)

where the symbols are the same as in equation (9). When the sum of gravitational and repulsive forces is the minimum, the individual density of components reaches the peak value, and the derivative of the sum of repulsive and gravitational forces is 0. Therefore, *I* can be calculated via

14 
$$I = \frac{c\gamma\sigma}{\tau\beta m} d^{*\sigma-\tau\beta}$$
(11)

15 The *G* value of the same type of component can be obtained by the geometric mean16 of the same component in multiple cities,

17  $G = (\prod_{i=1}^{N} G_i)^{1/N}$ (12)

18 where  $G_i$  is the constant of proportionality in city *i*, the value of which is obtained by 19 model fitting, and *N* is the number of the case cities.

The regression analysis showed that the  $d^*$  of a type of component was significantly related to the urban population of the 13 cities (*SI Appendix*, Fig. S4). Then *I* can be derived from  $d^*$ , which is determined by the gravitational and repulsive force. In order to

study the effects of city development on component distribution, the attributes of the latest period in Hangzhou and Ningbo were used to predict the distribution of KFC, ZTO and GH over time. The predictions matched the 3 components' distribution curves well  $(R^2 > 0.53, SI Appendix, Fig. S5).$ 

The magnitudes of the average G of KFC and ZTO located in urban areas are both  $10^{-12}$ , while the magnitudes of the average G of GH and DF located outside the city are  $10^{-6}$  and  $10^{-8}$  respectively. The difference in the G values of components inside and outside the city is of 4-6 orders of magnitude (*SI Appendix*, Table S4).

9 We predict the individual density curves of the four types of components in the other two cities (Wuhan and Nanjing City) according to the relationships between the model 10 11 parameters and the attributes in 13 cities (SI Appendix, Fig. S4). The predicted curves match well (P < 0.05) with the real-world data of the distribution of components 12 (respectively, SI Appendix, Fig. S6). The predictions validate the universality of the 13 14 model among different cities (SI Appendix, Tables S5-6). Furthermore, the gradient model 15 could be extend to simulates many types of components co-exist in an urban-rural system 16 (SI Appendix, Fig. S7).

17

#### 18 Discussion

John von Neumann used to say, "with four parameters I can fit an elephant" (29). It means that excessive arbitrary parameters made model loss the significance. Fortunately, our gradient model has only one arbitrary parameter *G*, and the other two parameters *I* and *Z*, can be calculated from real-world data (*SI Appendix*, Fig. S4). The parameters used in the gradient model are easy to observe and calculated, and the simulation results

can be verified by filed investigations. It means that our gradient model is reliable and 1 robust, for it stands on the solid ground of physics. Former models mainly consider the 2 3 two-dimensions mainly identify 'islands' or 'lowlands' in urban area for some parameters (9). Their data and analysis can easily be transformed and apply this 1-Dimesional 4 gradient model and quantify the relevant variables of spatial distribution of components, 5 including the economic revenue, population distribution and ecological preference. For 6 example, this 1-dimesional gradient model can provide a quantitative demonstration to 7 Christaller's central hypothesis (30). Urban planners can use this model to accurately 8 predict how cities will develop over time, by consider the changes of population, land 9 rent and ecological consciousness. 10

11 The sensitivity analysis of the gradient model shows that the distributions of multiple types of components are more sensitive to four input parameters, m, y,  $\sigma$  and r, 12 than other parameters. These four parameters largely determine the gravity and repulsion 13 14 forces (SI Appendix, Table S7). It means that the attributes of components together with 15 the attributes of cities jointly determine the functional spatial structure of cities. The 16 attributes of components include net ecosystem service (m) and environmental index  $(\gamma)$ , 17 and the attributes of cities include land rent exponent ( $\sigma$ ) and population attenuation coefficient ( $\beta$ ). Many researchers find that the land rent and freight rate affect the 18 19 distribution of components (21), but few models quantify the affections. This 1-20 dimesional gradient model quantifies the influence of driving factors and find out the key factors. For example, the ecosystem service intensity m of greenhouses is much smaller 21 than that of KFCs, so it cannot afford the high land rent, therefore they are repulsed by 22 23 the city center. Meanwhile, the fresh-keeping distance r of greenhouse products is longer

than that of KFCs, so they are less attracted by the city center. The equilibrium of the two
forces mainly drives those greenhouses locate outside urban areas and far from other
functional components.

The gradient model uncovers the social-economic and ecological mechanism of 4 development of city's functional structure. The technological innovations of the 5 components increase the productivity *m* while decreasing the environmental impact  $\gamma$  of 6 the components. The improvements of the net benefit (combined m and y) of the 7 components raise the gravitation force to the components and then uplift the individual 8 density peak  $(P_{max})$  of the individuals and pull the  $P_{max}$  to move inward  $(d^* \text{ decreases})$  on 9 urban-rural gradients. (SI Appendix, Fig. S8). These results support the view that the 10 11 enterprises (city functional components or organaras) have to keep up with technological 12 innovations continuously (12, 31). Furthermore, the individual density curve response of 13 to the environmental index  $\gamma$  reveals that innovations must also reduce the environmental 14 impact of components in order to adapt to the changes in human preference, which tends 15 to be stricter on environment quality with increasing social prosperity (32, 33). The 16 super-cell city model has analyzed the spatial relationships between organaras and 17 citynucleus (6). The gradient model further quantifies the important impacts of the production capacity, ecological characteristics, and technological progress of organaras 18 19 on the city's functional spatial structure.

The land rent reflects the result of competition among components for a scarce land resource (28). The development of cities flattens the spatial patterns of land rent and human population (18). As the land rent curves become gentler, the  $P_{max}$  of the four types of components decrease, but only the  $d^*$  of GH and DF located outside the urban area

moves outward (SI Appendix, Table S7). In other words, the growth of population in the 1 peripheries of the city is caused by the urbanization (*SI Appendix*, Fig. S9b) will stimulate 2 3 the  $P_{max}$  of components move outward (SI Appendix, Fig. S8). The dynamics of cities, which include urbanization, counter urbanization, and re-urbanization, are essentially the 4 change of the city attributes (13). For example, the changes in economic level, population 5 size, urban area and structure (3, 9, 34). The change in total demand for the goods or 6 services of a type of component in a city (M) reflects the dynamics of the population and 7 its preferences, and it affects the  $P_{max}$ . The city index Z, which is highly related to the 8 9 maximum land rent and the size of the city's urban area (*SI Appendix*, Fig. S4), enhances the  $P_{max}$  but maintains the position of  $d^*$  (SI Appendix, Fig. S8). Through above 10 11 mechanism, the gradient model could help us to quantify the self-organization processes of a eukarcity, including coexistence of and competition between different types of 12 organaras revealed by Chang et al. 2021 (6). The mechanism could be the basis for 13 14 predicting the future city structure based on the city's attributes along with the 15 development of cities.

16 Although each case city has its unique spatial structure and development trend, the 17 gradient model in this study has been proven the generality to analyze the spatial distribution of city functional components. Actually, the key input parameters are the 18 19 spatial distribution function of human population and land price and the component 20 production capacity. We consider that the model has the potential to apply in other cities around the world. On the one hand, we have found the trends of land rent curve and 21 population density curve along the urban-rural gradient of some cities in the United 22 23 States, Japan, South Korea, Australia and Europe are similar to the patterns of the Chines

1 cities, and it shows the monotonic attenuation trend from city center outward (18,35). On the other hand, recent studies have shown that the affluent population mainly occupies 2 3 the position of urban center, even in mega cities such as New York and London (36) that similar to the case Chinese cities in this study. Although some rich people tent to live in 4 the outer suburbs, the small population cannot change the spatial pattern of high 5 accessibility of urban center. Therefore, once the input parameters were obtained, the 6 model could be used to describe the distribution pattern of functional components in 7 other cities worldwide. In the future, the studies can be carried out across regions and 8 countries for comparing the similarities and differences of diverse cities and countries, 9 and reveal the principle behind the phenomenon. 10

11 This model integrates the various factors and their interactions into a one-dimensional urban-rural gradient and finds quantified rules. This static model describes the interaction 12 13 results of various factors as the eco-economic system in relative equilibrium state. Such a 14 mechanism model, instead of the statistic model (7), reveals the general law of the 15 development, expansion, and renewal of the cities. This mathematical gradient model 16 deepens the understanding of city structure based on a conceptual super cell model (6). 17 Based on the historical distributions of the functional components and related parameters, the model can be used to predict the development the city morphology and structure. The 18 model can also help to explore the limitations of the current city in structure and function, 19 20 and to find out the crucial optimization points to promote sustainable development in the context of global urbanization. It can be further developed and inspire interdisciplinary 21 studies across fields such as ecology, economics, urban planning and management, and 22 23 engineering.

1

#### 2 Materials and Methods

#### **3** Selection of case cities and functional components

The criteria for choosing case cities: (1) the data for the population and spatial 4 pattern of population of the city is available; (2) the data for the spatial pattern of land 5 price of the city is available; (3) a city is self-sustainable with complete processes and 6 function. According to the criteria, we selected 15 cities in China: Shanghai, Beijing, 7 Tianjin, Suzhou, Wuhan, Hangzhou, Nanjing, Wuxi, Ningbo, Nantong, Hefei, 8 Changzhou, Shaoxing, Jiaxing, and Zhenjiang City, and several time periods in some 9 cities (SI Appendix, Table S1). The criteria for choosing the type of component: (1) the 10 11 function of the components is to provide services to people locally, so their amount is related to the population of the city; (2) each component has a number of individuals that 12 13 form an individual density distribution curve along the urban-rural gradient; (3) different 14 types of components have distinguishable distribution curves along the urban-rural 15 gradient: one type is concentrated near the citynucleus, one type outside the center, one 16 type is near the urban fringe, and one is in the ex-urban area. According to the criteria, we 17 chose: (1) a type of fast food restaurant, Kentucky Fried Chicken shop (KFC), most of which are near the citynucleus; (2) a type of express delivery outlets, ZTO delivery 18 19 outlets, most of which are outside the citynucleus, (3) a primary biological production 20 component, cultivated greenhouses, which are mainly outside but near the suburban area, (4) a type of secondary biological production component, dairy farms, that are mainly 21 located in ex-urban areas (SI Appendix, Fig. S10). 22

#### **1** Data source and ecosystem services assessment

2 The data of city attributes and functional components are obtained by investigation 3 or public database, the details see Supplementary Information. Through the surveying and mapping of the land price of cities, it is found that there are still a large number of single-4 center cities. Of course, the research on multi-center cities may be disturbed, and needs 5 further study. According to the Millennium Ecosystem Assessment, ecosystem services 6 include provisioning services, regulating services, cultural services, and supporting 7 services (37). In this study, the ecosystem services (goods and services) provided by 8 9 artificial ecosystems (components) are divided into target services and accompanied 10 services separately (SI Appendix, Fig. S11) (7). The calculations of the ecosystem 11 services of the components see Supplementary Information. 12 The target services of a type of component are determined by the investment goal of 13 the artificial ecosystem. This means that they can be the provisioning, regulating, or 14 cultural services in Millennium Ecosystem Assessment (37). The target service of KFC, 15 greenhouses, and dairy farms is the provisioning of food, which is equivalent to some of 16 the provisioning services of natural ecosystems, while the target service of ZTO is the 17 regulating service of distributing goods to people. The accompanied services are equivalent to the externalities (positive or negative) in economics. They can be 18 19 categorized into provisioning, regulating or cultural services. Regulating services are 20 further divided into positive (services) and negative (dis-services) in this paper, following

The net service (NES, *m* in model) is the sum of the ecosystem services (target
 service + positive regulating services + cultural services) and dis-services (environmental

the guidelines in Liu et al. (38).

1 impacts),

$$NES = \sum_{i=1}^{n} ES_i \tag{13}$$

3 where  $ES_i$  (USD m<sup>-2</sup> yr<sup>-1</sup>) is the value of ecosystem service *i*, and *n* is the number of 4 ecosystem services considered in this study.

5 Environmental index (γ in model) is calculated by the ratio of target goods and
6 services (TGS) to dis-services (EDS) of a type of component,

$$\gamma = |EDS| / TGS \tag{14}$$

8

7

2

#### 9 Statistics

10 The statistic functions for the attributes of cities and components with distance from 11 the citynucleus uses linear and nonlinear regressions (Excel 2019, Microsoft 12 Cooperation). Linear and nonlinear regressions were used to study the relationship 13 between Z and the city attributes, and the best adjusted  $R^2$  was used to select the 14 regression form.

The nonlinear fitting module in Origin 2018 Pro (OriginLab Corporation) was used 15 to simulate the spatial distribution of functional components. As the initial values of 16 nonlinear fitting parameters may affect the simulation results, we carefully cycle through 17 the appropriate initial values. At the beginning of the model iterative process, we use the 18 19 default value of 1 as the initial value for G and I. Meanwhile, we fix Z as 0, because Z only affects the  $P_{max}$  without the peak position. After the model iteration is over at this 20 stage, we relax the condition on Z and continue with the iterative process to obtain the 21 22 final fitting parameters.

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8	R.X., K.H.C. analyzed the data; B.X., W.L. undertook the economic analysis; J.C., Y.G.,
9	G.Y. and K.H.C. wrote the manuscript. All authors performed research and approved the
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11	
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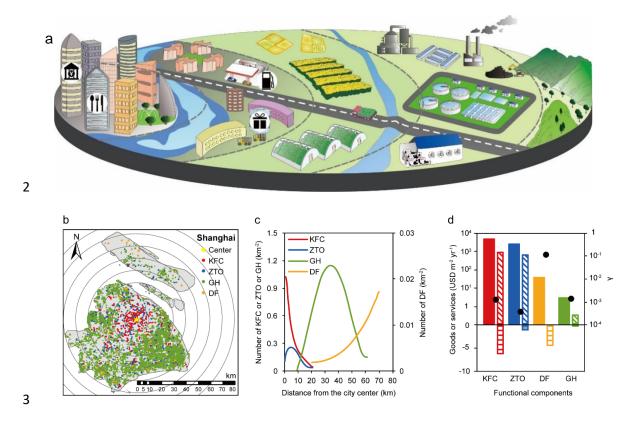
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### **1** Figures and Tables



4 Figure 1. A city's layout indicated by functional components. a, Illustration of multiple types of components distributed from citynucleus to rural area; b, two-5 6 dimensional pattern of four types of components in Shanghai City, KFC-Kentucky Fried 7 Chicken shops, ZTO-ZTO express outlets, GH-greenhouses, DF-dairy farms; c, onedimensional individual density curves of the four types of components along the urban-8 9 rural gradient; **d**, ecosystem services of the four types of components, solid bar: target services, diagonal bar: accompanied services, horizontal bar: dis-services, black points: y 10 (absolute value of the ratio of dis-service/target services) of the components. 11 12

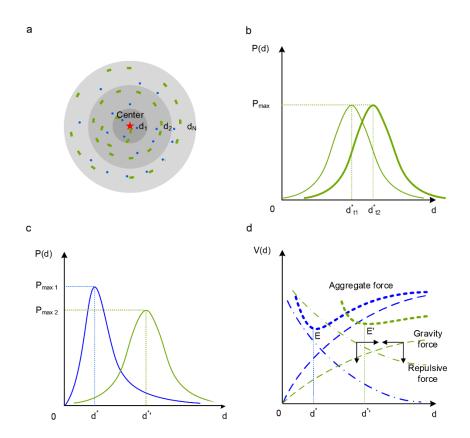




Figure. 2. Model hypothesis for the mechanism of the spatial distribution of city 2 3 components. a, In an ideal city, the two-dimensional distribution patterns of population and functional components obtain their highest individual density at the center and 4 5 become sparser farther out. The colors of the points indicate the different types of components, and the colors of the ring from dark to gray indicate the human population 6 density from high to low; **b**, location of the individual density peak  $(P_{max})$  of one type of 7 component shifts along the urban-rural gradient ( $d^*_{t1}$  to  $d^*_{t2}$ ) with time; **c**, the distribution 8 of two types of components along the urban-rural gradient. The  $d^*$  and  $d^{*'}$ 9 of  $P_{max}$ correspond to the locations of E and E' in Fig. 2d, colors of lines correspond to the 10 types of components in Fig. 2d; d, repulsive force (dash-dotted line) and reverse gravity 11 12 force (thin dashed line) for components on an urban-rural gradient, the thick dashed lines

show the aggregate forces, and the colors of the lines are corresponding to the types of
 components in Fig. 2a, *E* and *E*' are the minimum aggregate forces, and arrows indicate
 the directions in which forces act on the components.

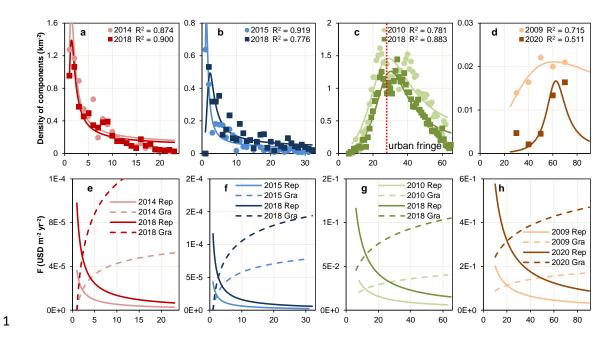


Figure. 3. Simulated individual density curves of the components and the driven forces in Shanghai City in two periods. a-d, Simulated individual density curves and real-world data of the four types of components along the urban-rural gradient: a, Kentucky Fried Chicken shops; b, ZTO Express outlets; c, cultivated greenhouses, red dotted line indicates the location of the urban fringe; d, dairy farms; e-h, the repulsive force (solid line) and the reverse-gravitational force (dashed line) of the components correspond to a-d, respectively.

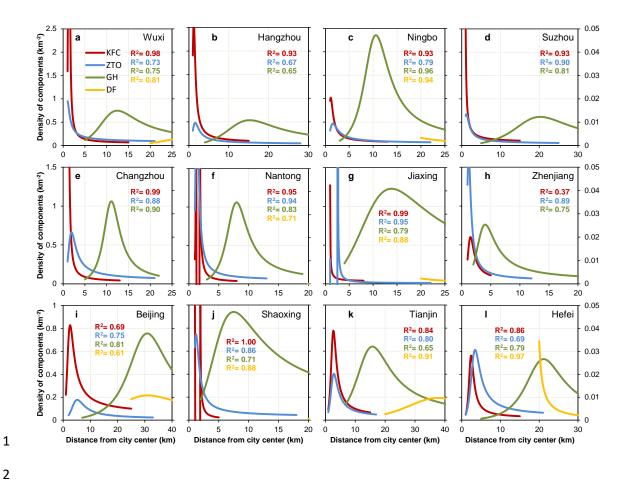




Figure. 4. Simulated spatial distribution of 4 types of components in 12 case cities. 3 4 The individual density of Kentucky Fried Chicken shops (KFCs), ZTO Express outlets and cultivated greenhouses (GHs) correspond to the left axis while dairy farms (DFs) 5 correspond to the right axis. Note the DFs are few in some cities and non-existent in 6 some other cities. The number of KFCs in Shaoxing City and Nantong City and the 7 number of ZTOs in Jiaxing City are too few to be simulated. For the real-world data, see 8 9 SI Appendix, Fig. S1.