Adrian Bejan
Gilbert W. Merkx
*Editors*

# Constructal Theory of Social Dynamics

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# Chapter 11
# Statistical Mechanical Models for Social Systems

Carter T. Butts

## 11.1. Summary

In recent years, researchers in the area of constructal theory have sought to apply principles from the modeling of engineered systems to problems throughout the sciences. This chapter provides an application of statistical mechanical models to social systems arising from the assignment of objects (e.g., persons, households, or organizations) to locations (e.g., occupations, residences, or building sites) under the influence of exogenous covariates. Two illustrative applications (occupational stratification and residential settlement patterns) are presented, and simulation is employed to show the behavior of the location system model in each case. Formal analogies between thermodynamic and statistical interpretations of model elements are discussed, as is the compatibility of the location system model with the assumption of stochastic optimization behavior on the part of individual agents.

## 11.2. Introduction

At their core, developments in the growing body of literature known as "constructal theory" (Bejan 1997, 2000; Bejan and Lorente 2004; Bejan and Marden 2006; Reis and Bejan 2006) reflect an effort to apply principles from the modeling of engineered systems to problems throughout the sciences. In this respect, constructal theory falls within the tradition of researchers such as Zipf (1949) and Calder (1984), who have sought to capture the behavior of a diverse array of systems via a combination of physical constraints and optimization processes. Within the social sciences, constrained optimization has been central to research on choice theoretic models (the dominant paradigm in economics) and has had a strong influence on the literatures in organization theory (particularly organizational design) and human judgment and decision making. While optimization-based models have not always proven correct, their simplicity and generalizability continue to attract interest from researchers in many fields. In contrast, physical constraints – or even models borne of physical processes – have seen only intermittent integration into social science research. This is unfortunate, given both the reality of physical limits on social organization and the potential applicability of certain physical models to social systems.* Here, we describe one modeling framework which incorporates both elements to capture the behavior of high-dimensional social systems whose components exhibit complex dependence. Although inspired by related models within social network analysis, this framework can be shown to admit a physical interpretation, thereby facilitating the application of insights from other fields (particularly statistical mechanics) to a broad class of social phenomena. It is hoped that the results shown here will serve to encourage further development of social models which capitalize on analogies with physical processes.

### *11.2.1. Precursors Within Social Network Analysis*

A fundamental problem facing researchers in the social network field has been the need to model systems whose elements depend upon one another in non-trivial ways. For instance, in modeling directed relations (i.e., those with distinct senders and receivers), it will generally be the case that ties (or "edges," in the language of graph theory) sharing the same endpoints will depend upon one another. This form of dependence (called *dyadic dependence*) was combined with the notion of heterogeneity in rates of tie formation to form the first family of what would eventually be called *exponential random graph models*, the $p_1$ family (Holland and Leinhardt 1981). While dyadic dependence was relatively simple in nature, the models created to cope with it were rapidly expanded into more complex cases. For instance, Frank and Strauss (1986) famously considered graph processes in which two edges are dependent if they share any endpoint; this lead to the *Markov graphs*, whose properties are far more intricate than those of processes exhibiting only dyadic dependence. Extensions to other, still more extensive forms of dependence followed (e.g., Strauss and Ikeda 1990; Wasserman and Pattison 1996; Pattison and Wasserman 1999; Robins et al. 1999; Pattison and Robins 2002), along with corresponding innovations in simulation and inferential methods (Crouch et al. 1998; Snijders 2002; Hunter and Handcock 2006).

For our present purposes, it is important to emphasize that these developments did not arise from efforts within the social network field alone. Rather, they resulted from an interdisciplinary synthesis in which insights from areas such as spatial statistics (e.g., Besag 1974, 1975) and statistical physics (Strauss 1986; Swendsen and Wang 1987), as well as innovations in computing technology and simulation methods (Geyer and Thompson 1992; Gamerman 1997), were leveraged to formulate and solve problems within the social sciences. In the best tradition of such "borrowing," scientific advances were made neither by ignoring external developments nor by blindly importing models from other disciplines (nor still by an "invasion" of scientists from these disciplines into the network field). Progress resulted instead from the recognition of structural similarities between problems in network research and problems in other substantive domains, followed by the adaptation and translation of models from these fields into the network context. This approach has allowed network researchers to avoid many of the pitfalls identified by Fararo (1984) associated with the importation of mathematically attractive models with poor empirical motivation. It may also serve as a useful example to be emulated by workers in areas such as constructal theory, who seek to apply their ideas to novel substantive domains.

While the focus of this chapter is not on network analysis, the approach taken here owes much to the exponential family modeling tradition described above. It also draws heavily on the statistical mechanical framework to which that tradition is closely related. More specifically, this chapter presents a family of models for social phenomena which can be described in terms of the arrangement of various (possibly related) objects with respect to a set of (again, possibly related) locations. This family is designed so as to leverage the large literature on the stochastic modeling of systems with non-trivial dependence structures. It is also constructed so as to be applicable across a wide range of substantive contexts; to scale well to large social systems; to be readily simulated; to be specifiable in terms of directly measurable properties; and to support likelihood-based inference using (fairly) standard methods. Although this model family is not obviously "constructal" in the sense of Bejan (1997, 2000), it does incorporate elements of (local) optimization and physical constraint. Thus, it may be of some interest to those working in the area of constructal theory per se.

The structure of the remainder of the chapter is as follows. After a brief comment on notation, we present the core formalism of the chapter (the generalized location system). Given this, we turn to a discussion of modeling location systems, including both conceptual and computational issues. Finally, we illustrate the use of the location system model to examine two classes of processes (occupational stratification and residential settlement patterns), before concluding with a brief discussion.

### *11.2.2. Notation*

We here outline some general notation, which will be used in the material which follows. A graph, G, is defined as $G = (V, E)$, where V is a set of vertices and E is a set of edges on V. When applied to sets, $|\cdot|$ represents cardinality; thus $|V|$ is the number of vertices (or order) of G. In some cases (particularly when dealing with valued graphs), it will be useful to represent graphs in adjacency matrix form, where the adjacency matrix X for graph G is defined as a $|V| \times |V|$ matrix such that $X_{ij}$ is the value of the (i, j) edge in G. By convention, $X_{ij} = 0$



* Recognition of this connection is at least as old as the founding of sociology, which was initially envisioned as leading to a form of "social physics" (Quetelet 1835, Comte 1854). Although primarily invoked for rhetorical purposes, this stance foreshadowed later developments such as the work of Coleman (1964), who drew extensively on physical models.

if G contains no (i, j) edge. A tuple of graphs $(G_1, \ldots, G_n)$ on common vertex set V may be similarly represented by a $n \times |V| \times |V|$ adjacency array, X, such that $X_{ij}$ is the adjacency matrix for $G_i$.

When referring to a random variable, X, we denote the probability of a particular event x by $\Pr(X = x)$. More generically, $\Pr(X)$ refers to the probability mass function of X (where X is discrete). Expectation is denoted by the operator $\mathbf{E}$, with subscripts used to designate conditioning where necessary. Thus, the parametric pmf $\Pr(X|\theta)$ leads to the corresponding expectation $\mathbf{E}_\theta(X)$. (Likewise for variance, written $\mathrm{Var}_\theta(X)$.) When discussing sequences of realizations of a random variable X, parenthetical superscript notation is used to designate particular draws (e.g., $(x^{(1)}, \ldots, x^{(n)})$). Distributional equivalence is denoted by $\sim$ (read: "is distributed as"), so $X \sim Y$ implies that X is distributed as Y. For convenience, this notation may also be extended to pmfs, such that $X \sim f$ (for random variable X and pmf f) should be understood to mean that X is distributed as a random variable with pmf f.

## 11.3. Generalized Location Systems

Our focus here is on what we shall call *generalized location systems*, which represent the allocation of arbitrary entities (e.g., persons, objects, organizations) to "locations" (e.g., physical regions, jobs, social roles). While our intent is to maintain a high level of generality, we will limit ourselves to systems for which both entities and locations are discrete and countable, and for which it is meaningful to treat the properties of entities and locations as relatively stable (at least for purposes of analysis). Relaxation of these constraints is possible, but will not be discussed here; even with these limitations, however, the present framework still allows for a great deal of flexibility.

We begin by positing a system of n identifiable *objects*, $O = (o_1, \ldots, o_n)$, each of which may reside in exactly one of m identifiable *locations*, $L = (l_1, \ldots, l_m)$. The state of this system at any given time is represented by a *configuration vector*, $\ell \in \{1, \ldots, m\}^n$, which is defined such that $\ell_i = j$ iff $o_i$ resides at location $l_j$. Depending on the system in question, not all hypothetical configuration vectors are physically realizable; the set of all such realizable vectors is said to be the set of *accessible configurations*, and is denoted $\mathbb{C}$. $\mathbb{C}$ may be parameterized in a number of ways, perhaps the most important of which being in terms of *occupancy constraints*. We define the *occupancy function* of a location system as

$$\mathbf{P}(x, \ell) = \sum_{i=1}^{n} I(\ell_i = x), \tag{11.1}$$

where I is the standard indicator function. The vectors of maximum and minimum occupancies for a given location system are composed of the maximum/minimum values of the occupancy function for each state under $\mathbb{C}$ (respectively). That is, we require that $P_i^- \leq \mathbf{P}(i, \ell) \leq P_i^+$ for all $i \in 1, \ldots, m$, $\ell \in \mathbb{C}$, where $P^-$, $P^+$ are the minimum and maximum occupancy vectors. If $P_i^- = P_i^+ = 1 \;\; \forall \;\; i \in 1, \ldots, m$, then it follows that $\ell$ is a permutation vector on $1, \ldots, n$, in which case we must have $m = n$ for non-empty $\mathbb{C}$. This is an important special case, particularly in organizational contexts (White 1970). By contrast, it is frequently the case in geographical contexts (e.g., settlement) that $P_i^- = 0$ and $P_i^+ > n \;\; \forall \;\; i \in 1, \ldots, m$, in which case occupancy is effectively unconstrained.



In addition to configurations and labels, objects and locations typically possess other properties of scientific interest. We refer to these as *features*, with $F_O$ being the set of object features and $F_L$ being the set of location features. While we do not (initially) place constraints on the feature sets, it is worth highlighting two feature types which are of special interest. Feature vectors provide ways of assigning numerical values to individual objects or locations, e.g., age, average rent level, or wage rate. Adjacency matrices can also serve as important features, encoding dyadic relationships among objects or locations. Examples of such relationships can include travel distance, marital ties, or demographic similarity. Because relational features allow for coupling of objects or locations, they play a central role in the modeling of complex social processes (as we shall see).

To draw the above together, we define a generalized location system by the tuple $(L, O, \mathbb{C}, F_L, F_O)$. The state of the system is given by $\ell$, which will be of primary modeling interest. Various specifications of $\mathbb{C}$ are possible, but particular emphasis is placed on occupancy constraints, which specify the range of populations which each location can support. With these elements, it is possible to model a wide range of social systems, and it is to this problem that we now turn.

## 11.4. Modeling Location Systems

Given the definition of a generalized location system, we now present a stochastic model for its equilibrium state. In particular, we assume that – given a set of accessible configurations, $\mathbb{C}$– the system will be found to occupy any particular configuration, $\ell$, with some specified probability. Our primary interest is in the modeling of these equilibrium probabilities, although some dynamic extensions are possible.

Given the above, we first define the set indicator function

$$I_{\mathbb{C}}(\ell) = \begin{cases} 1 & \text{if } \ell \in \mathbb{C} \\ 0 & \text{otherwise} \end{cases} \tag{11.2}$$

The equilibrium probability of observing a given configuration can then be written as

$$\Pr(S = \ell) = I_{\mathbb{C}}(\ell) \frac{\exp(P(\ell))}{\sum_{\ell' \in \mathbb{C}} \exp(P(\ell'))} \tag{11.3}$$

where S is the random state, and P is a quantity called the *social potential* (defined below). The sum

$$Z(P, \mathbb{C}) = \sum_{\ell' \in \mathbb{C}} \exp(P(\ell')) \tag{11.4}$$

is the *normalizing factor* for the location model, a quantity which corresponds directly to the partition function of statistical mechanics (Kittel and Kroemer 1980). Equation (11.3) defines a discrete exponential family on the elements of $\mathbb{C}$, and is complete in the sense that any pmf on $\mathbb{C}$ can be written in the form of Eq. (11.3). This completeness is an important benefit of the discrete exponential family framework, but there are other benefits as well. For instance, models of this type have been widely explored in both physics and mathematical statistics (see, e.g., Barndorff-Nielsen 1978; Brown 1986), facilitating the cross-application of existing knowledge to new modeling problems. Also significant is the fact that, for appropriate parameterizations of P, a number of well-known results allow for likelihood-based inference of model parameters from empirical data (Johansen 1979). These advantages may be contrasted with, for instance, those of intellective agent-based approaches, which (while dynamically flexible) frequently exhibit poorly understood behavior, and which rarely admit a principled theory of inference.

While Eq. (11.3) can represent any distribution on $\mathbb{C}$, its scientific utility clearly lies in identifying a theoretically appropriate specification of P. Intuitively, the social potential for any given configuration is equal to its log-probability, up to an additive constant. Thus, the location system is more likely to be found in areas of high potential, and/or (in a dynamic context) to spend more time in such states. While any number of forms for P could be proposed, we here work with a constrained family which incorporates several features of known substantive importance for a variety of social systems. This family of potential functions is introduced in the following section.

### 11.4.1. A Family of Social Potentials

As noted above, we seek a family of functions $P : \mathbb{C} \mapsto \mathbb{R}$ such that $\Pr(S = \ell) \propto \exp(P(\ell))$. This family should incorporate as wide a range of substantively meaningful effects as possible; since it is not reasonable to expect effects to be identical in every situation, the family should be *parameterized* so as to allow differential weighting of effects. Ideally, the social potential family should also be easily computed, and its structure easily interpreted.

An obvious initial solution to this problem is to construct P from a linear combination of deterministic functions of $F_L$ and $F_O$, which then act as sufficient statistics for the resulting distribution. Employing such a potential function within Eq. (11.3) leads to a regular exponential family on $\mathbb{C}$ (Johansen 1979), which has a number of useful statistical implications. The so-called "curved" exponential family models (which are formed by allowing P to be a non-linear function of statistics and parameters) (Efron 1975) are also possible, and may be useful in certain cases (e.g., where one must enforce a functional relationship among large numbers of parameters; see Hunter and Handcock 2006, for a network-related example). Here, we restrict ourselves to the linear case.



Even if a linear form is supposed, however, we are still left with the question of which effects should be included in the social potential. By definition, these effects must be parameterized as functions of the location and object features. Further, both location and object features (as we are using the term) can include both attributes (features of the individual location or object per se) and relations (features of object or location sets). Here, we will limit ourselves to relations which are dyadic (i.e., defined on pairs) and single-mode (i.e., which do not mix objects and locations). Thus, our effects should be functions of feature vectors, and/or (possibly valued) graphs.

While this constraint still admits a wide range of possibilities, we can further focus our attention by noting that the purpose of P is ultimately to control the assignment of objects to locations. This suggests immediately that the effects of greatest substantive importance will be those which draw objects toward or away from particular locations. Table 11.1 provides one categorization of such effects by feature type. In the first (upper left) cell, we find effects which express direct attraction or repulsion between particular objects and locations, based on their attributes. In the second (upper right) cell are effects which express a tendency for objects linked through connected locations to be particularly similar or distinct. (Spatial autocorrelation is a classic example of such an effect.) The converse family of effects is found in the third (lower left) cell; these effects represent a tendency for objects to be connected to other objects with similar (or different) locations. Homophily in career choice—where careers are interpreted as "locations"—serves as an example of a location homogeneity effect. Finally, in the fourth (lower right) cell we have effects based on the tendency of location relations to align (or disalign) with object relations. Propinquity, for example, is a tendency for adjacent objects to reside in nearby locations.

Taken together, these four categories of effects combine to form the social potential. Under the assumption of linear decomposability, we thus posit four sub-potentials (one for each category) such that

$$P(\ell) = P_\alpha(\ell) + P_\beta(\ell) + P_\gamma(\ell) + P_\delta(\ell). \tag{11.5}$$

TABLE 11.1. Elements of the social potential

| | Location attributes | Location relations |
|---|---|---|
| Object Attributes | Attraction/Repulsion Effects | Object Homogeneity/ Heterogeneity Effects (through Locations) |
| Object Relations | Location Homogeneity/Heterogeneity Effects (through Objects) | Alignment Effects |

We now consider each of these functions in turn. The first class of effects which must be represented in any practical location system are global attraction/repulsion—also called "push/pull"—effects. Residential locations, potential firm sites, occupations, and the like have features which make them generally likely to attract or repel certain objects (be they persons, organizations, or other entities). Such effects are naturally modeled via product-moments of attributes. Let $Q \in \mathbb{R}^{m\times a}$, $X \in \mathbb{R}^{n\times a}$ be exogenous features reflecting location and object attributes (respectively), and let $\alpha \in \mathbb{R}^a$ be a parameter vector. Then we may define $P_\alpha$ as

$$P_\alpha(\ell) = \sum_{i=1}^{a} \alpha_i t_i^\alpha(\ell) \tag{11.6}$$

$$= \sum_{i=1}^{a} \alpha_i \sum_{j=1}^{n} Q_{\ell_j i} X_{ji}, \tag{11.7}$$

where $t^\alpha$ is a vector of sufficient statistics.

A second class of effects concerns object homogeneity/heterogeneity—that is, the conditional tendency for associated locations to be occupied by objects with similar (or different) features. Let $Y \in \mathbb{R}^{n\times b}$ be a matrix of object attributes, $B \in \mathbb{R}^{b\times m\times m}$ be an adjacency array on the location set, and $\beta \in \mathbb{R}^b$ a parameter vector. Then we define the object homogeneity/heterogeneity potential by

$$P_\beta(\ell) = \sum_{i=1}^{b} \beta_i t_i^\beta(\ell) \tag{11.8}$$

$$= \sum_{i=1}^{b} \beta_i \sum_{j=1}^{n} \sum_{k=1}^{n} B_{i\ell_j\ell_k} \left|Y_{ji} - Y_{ki}\right|, \tag{11.9}$$

where, as before, $t^\beta$ is a vector of sufficient statistics. It should be noted that the form of $t^\beta$ is closely related to Geary's C, a widely used index of spatial autocorrelation (Cliff and Ord 1973). $t^\beta$ is based on absolute rather than squared differences, and is not normalized in the same manner as C, but its behavior is qualitatively similar in many respects.

The parallel case to $P_\beta$ is $P_\gamma$, which models the effect location homogeneity or heterogeneity through objects. Let $R \in R^{m\times c}$ be a matrix of location features, $A \in \mathbb{R}^{c\times n\times n}$ be an adjacency array on the object set, and $\gamma \in \mathbb{R}^c$ be a parameter vector. Then $P_\gamma$ is defined as follows:

$$P_\gamma(\ell) = \sum_{i=1}^{c} \gamma_i t_i^\gamma(\ell) \tag{11.10}$$

$$= \sum_{i=1}^{c} \gamma_i \sum_{j=1}^{n} \sum_{k=1}^{n} A_{ijk} \left|R_{\ell_j i} - R_{\ell_k i}\right|, \tag{11.11}$$

As implied by the above, $t^\gamma$ is the vector of sufficient statistics for location homogeneity. $t^\gamma$ is at core similar to $t^\beta$, save in that the role of object and location are reversed: absolute differences are now taken with respect to *location* features, and are evaluated with respect to the connections between the objects occupying said locations.



The final element of the social potential is the alignment potential, $P_\delta$, which expresses tendencies toward alignment or disalignment of object and location relations. Given object and location adjacency arrays $W \in \mathbb{R}^{d\times n\times n}$ and $D \in \mathbb{R}^{d\times m\times m}$ (respectively) and parameter vector $\delta \in \mathbb{R}^d$, the alignment potential is given by

$$P_\delta(\ell) = \sum_{i=1}^{d} \delta_i t_i^\delta(\ell) \tag{11.12}$$

$$= \sum_{i=1}^{d} \delta_i \sum_{j=1}^{n} \sum_{k=1}^{n} W_{ijk} D_{i\ell_j\ell_k}, \tag{11.13}$$

where, as in the prior cases, $t^\delta$ represents the vector of sufficient statistics. The form chosen for $t^\delta$ is Hubert's Gamma, which is the standard matrix cross-product moment (see Hubert 1987, for a range of applications).

It should be noted that all four effect classes can actually be written in terms of matrix cross-product moment statistics on suitably transformed adjacency arrays, and hence only $P_\delta$ is formally required to express P. Although formally equivalent to that shown above, this parameterization obscures the substantive interpretation of matrix/vector effects outlined in Table 11.1, and requires pre-processing of raw adjacency data; for this reason, we will continue to treat the sub-potentials as distinct in the treatment which follows. Given this parameterization, we may complete our development by substituting the quantities of Eqs. (11.7–11.13) into Eq. (11.5) which gives us

$$P_{(\ell)} = \sum_{i=1}^{a} \alpha_i t_i^\alpha(\ell) + \sum_{i=1}^{b} \beta_i t_i^\beta(\ell) + \sum_{i=1}^{c} \gamma_i t_i^\gamma(\ell) + \sum_{i=1}^{d} \delta_i t_i^\delta(\ell) \tag{11.14}$$

in terms of sufficient statistics, or

$$\begin{aligned} P(\ell) = {} & \sum_{i=1}^{a} \alpha_i \sum_{j=1}^{n} Q_{\ell_j i} X_{ji} + \sum_{i=1}^{b} \beta_i \sum_{j=1}^{n} \sum_{k=1}^{n} B_{i\ell_j\ell_k} \left|Y_{ji} - Y_{ki}\right| \\ & + \sum_{i=1}^{c} \gamma_i \sum_{j=1}^{n} \sum_{k=1}^{n} A_{ijk} \left|R_{\ell_j i} - R_{\ell_k i}\right| + \sum_{i=1}^{d} \delta_i \sum_{j=1}^{n} \sum_{k=1}^{n} W_{ijk} D_{i\ell_j\ell_k} \end{aligned} \tag{11.15}$$

in terms of the underlying covariates. Together with Eq. (11.3), Eq. (11.15) specifies a regular exponential family of models for the generalized location system. As we have seen, this family allows for the independent specification of attraction/repulsion, heterogeneity/homogeneity, and alignment effects. Although motivated on purely social grounds, it is noteworthy that this model is fundamentally statistical mechanical in nature. Given the broader focus of this book on the application of physical modeling strategies to a wide range of substantive areas, we now consider this connection in greater detail.

## *11.4.2. Thermodynamic Properties of the Location System Model*

We have already seen that the stochastic location system model of Eq. (11.3) can be viewed as directly analogous to a standard class of statistical mechanical models. This fact allows us to employ some useful results from the physics literature (see, e.g., Kittel and Kroemer 1980) to elucidate several aspects of model behavior. (Interestingly, many of these results have parallels within the statistical literature, and can be derived in other ways; see, e.g., Barndorff-Nielsen (1978). See also Strauss (1986) for a similar discussion in the context of exponential random graph models.)

As noted above, the normalizing factor $Z(P, \mathbb{C})$ is directly analogous to the *partition function* of statistical mechanics. The quantity $F = -\ln Z(P, \mathbb{C})$, in turn, corresponds to the *free energy* of the location system. In a classical statistical mechanical system, the probability of observing the system in microstate j is given by

$$p_j = \frac{\exp(-\varepsilon_j/\tau)}{Z}, \tag{11.16}$$

where $\varepsilon_j$ is the microstate energy of j and $\tau$ is the temperature. Thus, the log-probability of microstate j is a linear function of the free and microstate energies:

$$\ln p_j = F - \frac{\varepsilon_j}{\tau}. \tag{11.17}$$

Returning to Eq. (11.3), it is immediately apparent that the social potential P plays the role of $-\varepsilon/\tau$. Indeed, inspecting Eq. (11.14) reveals an even closer correspondence: the realizations of the sufficient statistics associated with the elements of $t^\alpha$, $t^\beta$, $t^\gamma$, and $t^\delta$ are similar to microstate energies, and the corresponding parameters ($\alpha$, $\beta$, $\gamma$, and $\delta$) can be thought of as vectors of inverse temperatures. More precisely, each sufficient statistic is analogous to the energy function (or Hamiltonian) associated with a particular "mode" of $\ell$, just as the total microstate energy of a particle system might combine contributions from translational, rotational, and/or vibrational modes. The "energy" associated with a particular microstate, $\ell$, in each mode is given by the value of the sufficient statistic for that microstate (i.e., $t_i^\theta(\ell)$). As in the physical case, the log-probability of observing a particular realization of the location system can be expressed as a "free energy" minus a linear combination of microstate "energies" whose coefficients correspond to "inverse temperatures." While one does not conventionally encounter multiple temperatures in a physical system (although a close examination of parameters such as the chemical potential shows them to act as de facto temperature modifiers), we will find that this metaphor is useful in understanding the behavior of the location system. This point was foreshadowed by Mayhew et al. (1995), who invoked an "energy distribution principle" in describing the occurrence of naturally forming groups. The present model implements a notion of precisely this sort, for more general social systems. As exponential family models also have the property of maximizing entropy conditional on their parameters and sufficient statistics, these location system models can also be thought of as a family of *baseline models* in the sense of Mayhew (1984a).



In addition to providing insight into system behavior, the above relations are also helpful in deriving other characteristics. For instance, the average microstate energy of the system described by Eq. (11.16) is given by $dF/d\theta$, where $\theta = \tau^{-1}$. It follows for our purposes that

$$E_{(\alpha,\beta,\gamma,\delta)} t_i^\theta = \frac{-d \ln Z(P, \mathbb{C})}{d\theta_i}, \tag{11.18}$$

where $\theta_i$ represents any parameter of the system. Thus, expectations for arbitrary sufficient statistics can be obtained through the partition function. Second moments may be obtained in a similar manner: the Hessian matrix $\frac{-d^2F}{d\theta^2}$ yields the variance-covariance matrix for all sufficient statistics in the system. (In the physical case, this corresponds to the *energy fluctuation*, or the *variance in energy*.)

Moments of sufficient statistics are useful for a variety of purposes, but other statistical mechanical properties of the location system may also be of value. For instance, the "heat capacity" of the system for parameter $\theta_i$ is given by $\mathrm{Var}(t_i^\theta(\ell))\theta_i^2 = \left.\frac{-d^2F}{d\theta^2}\right|_{ii} \theta_i^2$. In the physical case, heat capacity reflects the capacity of a system to store energy (in the sense of the change in energy per unit temperature). Here, heat capacity for parameter $\theta_i$ reflects the sensitivity of the corresponding statistic $t_i^\theta$ to changes in the "temperature" $1/\theta_i$. For instance, if $\theta_i$ corresponds to a attraction parameter between income and gender, then heat capacity can be used to parameterize the income consequences of a weakening (or strengthening) of the attractive tendency within the larger system.

Using arguments similar to the above, it is possible to derive analogs to various other thermodynamic properties such as pressure and entropy (the latter also obtainable through information-theoretic arguments). While one must always be careful in interpreting such quantities, they may nevertheless provide interesting and useful ways of describing the properties of location systems. We will see some of the interpretational value of thermodynamic analogy below, when we consider some sample applications of the location system model; before proceeding to this, however, we turn to the question of how location system behavior may be simulated.

## *11.4.3. Simulation*

For purposes of both prediction and inference, it is necessary to simulate the behavior of the location system model for arbitrary covariates and parameter values. Generally, it is not possible to take draws from the location system model directly due to the large size of $\mathbb{C}$: except in very special cases, the computational complexity of calculating $Z(P, \mathbb{C})$ is prohibitive, and hence the associated probability distribution cannot be normalized. Despite this limitation, approximate samples from the location system model may be readily obtained by means of a Metropolis algorithm. Given that numerous accessible references on the Metropolis algorithm and other Markov chain Monte Carlo methods are currently available (see, e.g., Gamerman 1997; Gilks et al. 1996; Gelman et al. 1995), we will focus here on issues which are specific to the model at hand. Fortunately, the location system model is not especially difficult to simulate, although certain measures are necessary to ensure scalability for large systems.

To review, a Metropolis algorithm proceeds in the following general manner (see Gilks et al. 1996, for further details). Let S be the (random) system state. We begin with some initial state $\ell^{(0)} \in \mathbb{C}$, and propose moving to a candidate state $\ell^{(1)}$ which is generally chosen so as to be in a neighborhood of $\ell^{(0)}$. (Some additional constraints (e.g., detailed balance) apply to the candidate distribution, but these do not affect the results given here.) The candidate state is then "accepted" with probability $\min\left(1, \frac{\Pr(S=\ell^{(1)}|P,\mathbb{C})}{\Pr(S=\ell^{(0)}|P,\mathbb{C})}\right)$. If accepted, the candidate becomes our new base state, and we repeat the process for $\ell^{(2)}$. If rejected, $\ell^{(1)}$ is replaced by a copy of $\ell^{(0)}$, and again the process is repeated. This process constitutes a Markov chain whose equilibrium distribution (under certain fairly broad conditions) converges to the target distribution (here, $\Pr(S|P, \mathbb{C})$). It is noteworthy that this process requires only that the target distribution be computable up to a constant factor; this feature makes Metropolis algorithms (and related MCMC techniques) very attractive to those working with exponential family models (e.g., Strauss 1986; Snijders 2002; Butts 2006).

#### 11.4.3.1. The Location System Model as a Constrained Optimization Process

In addition to the application of analogies from physical systems, a central element of constructal theory is constrained optimization. In that regard it is interesting to note that the equilibrium behavior of the location system model can be shown to emerge from a choice process in which individual agents (here, our "objects") act to stochastically maximize a utility function, subject to constrained options. In particular, let $u(\ell)$ be the utility of configuration $\ell$ for each agent, and let us imagine that opportunities for agents to change location arrive at random times. When such an opportunity arises, the agent in question is able to choose between moving to a specified alternative location and remaining in place. If the move in question is utility increasing (i.e., if $u(\ell') > u(\ell)$ for a move leading to location vector $\ell'$), then the agent relocates. Otherwise, we presume that the agent has some chance of moving regardless, corresponding to $\exp[u(\ell') - u(\ell)]$. This can be understood as a form of bounded rationality, in which agents occasionally overestimate the value of new locations, or as arising from unobserved heterogeneity in agent preferences. Under fairly mild conditions regarding the distribution of movement opportunities (most critically, each agent must have a non-zero probability of having the opportunity to move to any given location through some move sequence in finite time), this process forms a Markov chain whose equilibrium distribution is proportional to u; indeed, it is a special case of the Metropolis algorithm, described above. Given this, it follows that the equilibrium behavior of such a system can be described by the location system model in the case for which $u = P$. While this is not the only dynamic system which gives rise to this equilibrium distribution, it is nevertheless sufficient to show that the location system model can arise from a process of constrained stochastic optimization. This constitutes another affinity with the constructal perspective, albeit an attenuated one (since the optimization involved is only approximate).



## 11.5. Illustrative Applications

The location system model can be employed to represent a wide range of social systems. This breadth of potential applications is illustrated here by means of two simple examples, one involving economic inequality and another involving residential segregation. Although both examples shown here are stylized for purposes of exposition, they do serve to demonstrate some of the phenomena which can be captured by the location system model.

### *11.5.1. Job Segregation, Discrimination, and Inequality*

Our first application employs the location system to model occupational stratification. We begin by positing a stylized "microeconomy" of 100 workers (objects), who are matched with 100 distinct jobs (locations) on a 1:1 basis. The population of workers is taken to consist of equal numbers of men and women, who are allocated at random into heterosexual couples such that all individuals have exactly one partner. To represent other individual features which may affect labor market performance, we also rank the workers on a single dimension of "human capital," with ranks assigned randomly in alternating fashion by gender. (Thus, males and females have effectively identical human capital distributions, and human capital ranks are uncorrelated within couples.) Like workers, jobs vary in features which may make them more or less desirable; here, we assign each job a "wage" (expressed in rank order), and group jobs into ten contiguous occupational categories. Thus, the top ten jobs (by wage) are in the first category, the next ten are in the second category, etc. While this setting is greatly simplified, it nevertheless allows us to explore basic interactions between occupational segregation, household effects, and factors such as discrimination. Elaborations such as hierarchical job categories, distinct unemployed states, additional job or worker attributes, and relaxations of 1:1 matching, could easily be employed to model more complex settings.

To examine the behavior of the location system model under different assignment regimes, we simulate model draws across a range of parameter values.

For instance, the first panel of Fig. 11.1 shows the mean male/female wage gap (i.e., the difference between mean male and female wages) under a model incorporating human capital and discrimination effects. Both effects are implemented as α parameters, and thus reflect general sorting tendencies; in particular, higher values of $\alpha_1$ (discrimination) reflect stronger tendencies to place males in high-wage occupations, while higher values of $\alpha_2$ (human capital) reflect stronger tendencies to place workers with high levels of human capital in high-wage occupations. At $\alpha_i = 0$, the corresponding tendency is fully inactive; $\alpha = (0, 0)$ is thus a random mixing model. Negative values of $\alpha_1$ indicate discrimination in favor of females (i.e., a tendency to place males in low-wage occupations); since human capital is unlikely to have a negative effect on earnings, negative $\alpha_2$ values are not considered. Within Fig. 11.1, each plotted circle corresponds to the outcome of a simulation at the corresponding coordinates. Circle area indicates the magnitude of the observed effect (mean gap for the left-hand panel, variance in wage gap for the right-hand panel) and shading indicates the mean direction of the gap in question (dark favoring males and light favoring females). For the simulation 500 coordinate pairs were chosen, and 1,000 MCMC draws taken at each pair (thinned from a full sample of 200,000 per pair, with a burn-in period of 100,000 draws). To speed convergence, all chains were run in parallel using a coupled MCMC scheme based on Whittington (2000), with state exchanges among randomly selected chain pairs occurring every 25 iterations. Coordinates were placed using a two-dimensional Halton sequence (Press et al. 1992), as this was found to produce more rapid convergence for the coupled MCMC sampler than a uniform grid (but covers the space more evenly than would a pseudo-random sample). As shown by the first panel of Fig. 11.1, increasing discrimination in favor of males ($\alpha_1 > 0$) or females ($\alpha_1 < 0$) generates a corresponding increase in the wage gap. This effect is persistent, but attenuates in the presence of strong human capital effects; since human capital is here uncorrelated with gender, selection on this dimension tends to "dampen out" the effects of discrimination. This is particularly clear in the second panel of Fig. 11.1, which shows that wage gap variance diminishes rapidly as the merit effect climbs. Thus, both the stratified and unstratified states arising in the upper portion of the parameter space are appreciably lower in variance than the unstratified region close to the origin, an effect which is not captured by the mean gap alone.

An interesting counterpoint to the purely inhibitory effect of additional α effects (here, human capital) on stratification is the impact of occupational segregation. To capture the latter effect, we replace the second α effect with a β effect expressing the tendency for jobs within the same occupational category to be more (or less) heterogeneous with respect to their gender composition. Negative $\beta$ effects act to inhibit heterogeneity, and hence model (in this context) the effect of occupational segregation. Positive $\beta$ values, by contrast, imply supra-random mixing (as might be produced, for instance, by an affirmative action policy). The results from simulations varying both effects are shown in Fig. 11.2 (simulations for Figs. 11.2 and 11.3 were performed in the same manner as those of Fig. 11.1). While discrimination continues to have its usual effect,

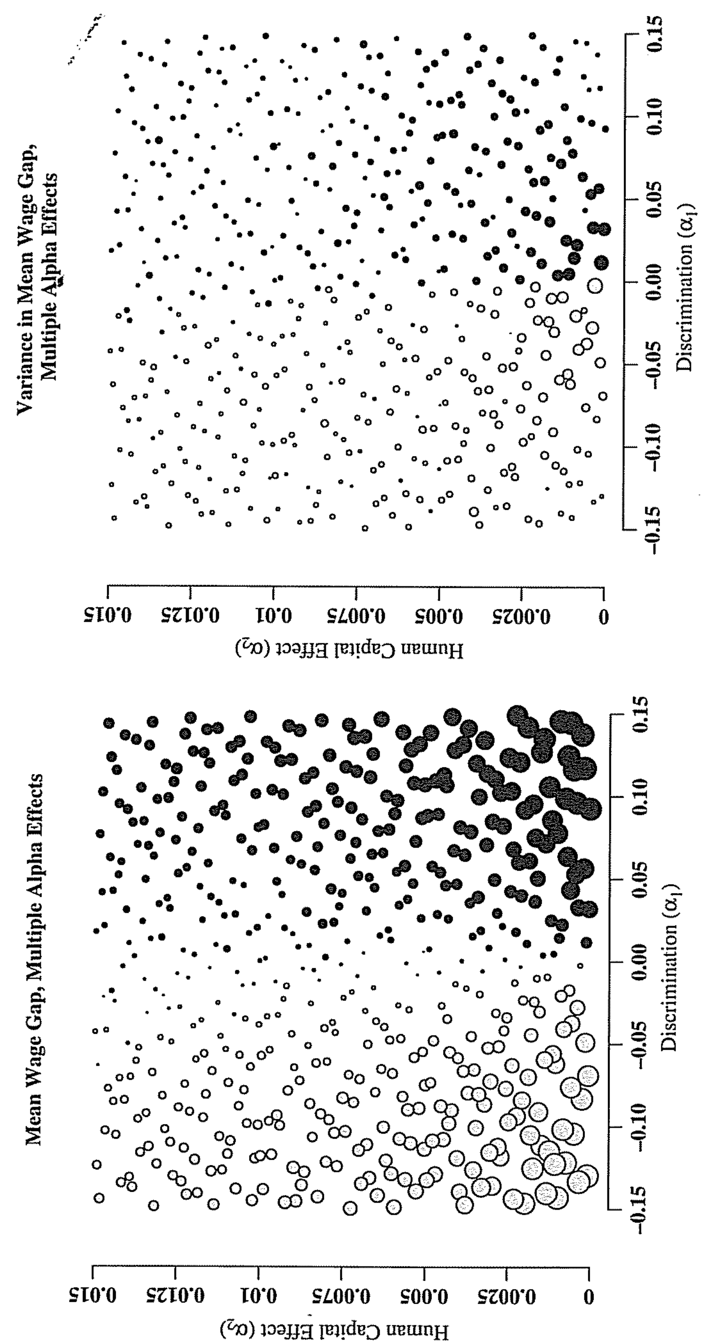


FIGURE 11.1. Gender difference in mean wage rank, discrimination, and human capital effects

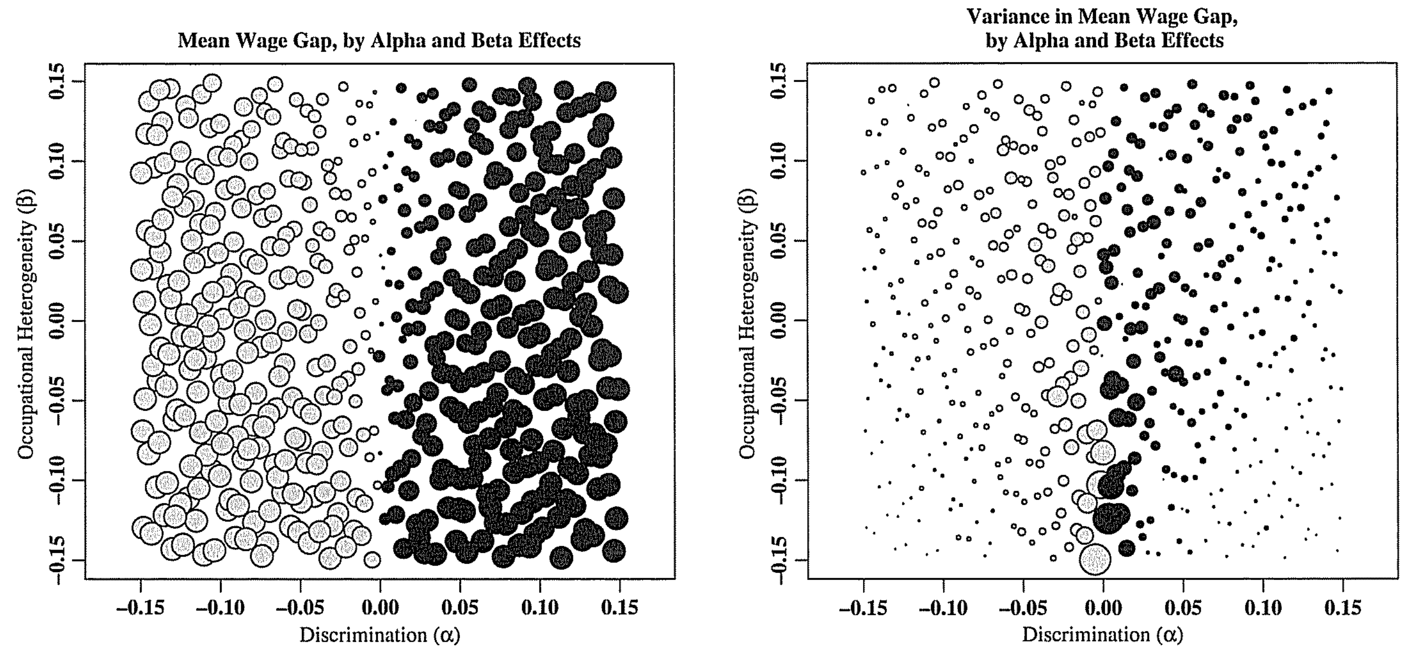


FIGURE 11.2. Gender difference in mean wage rank, discrimination, and segregation effects

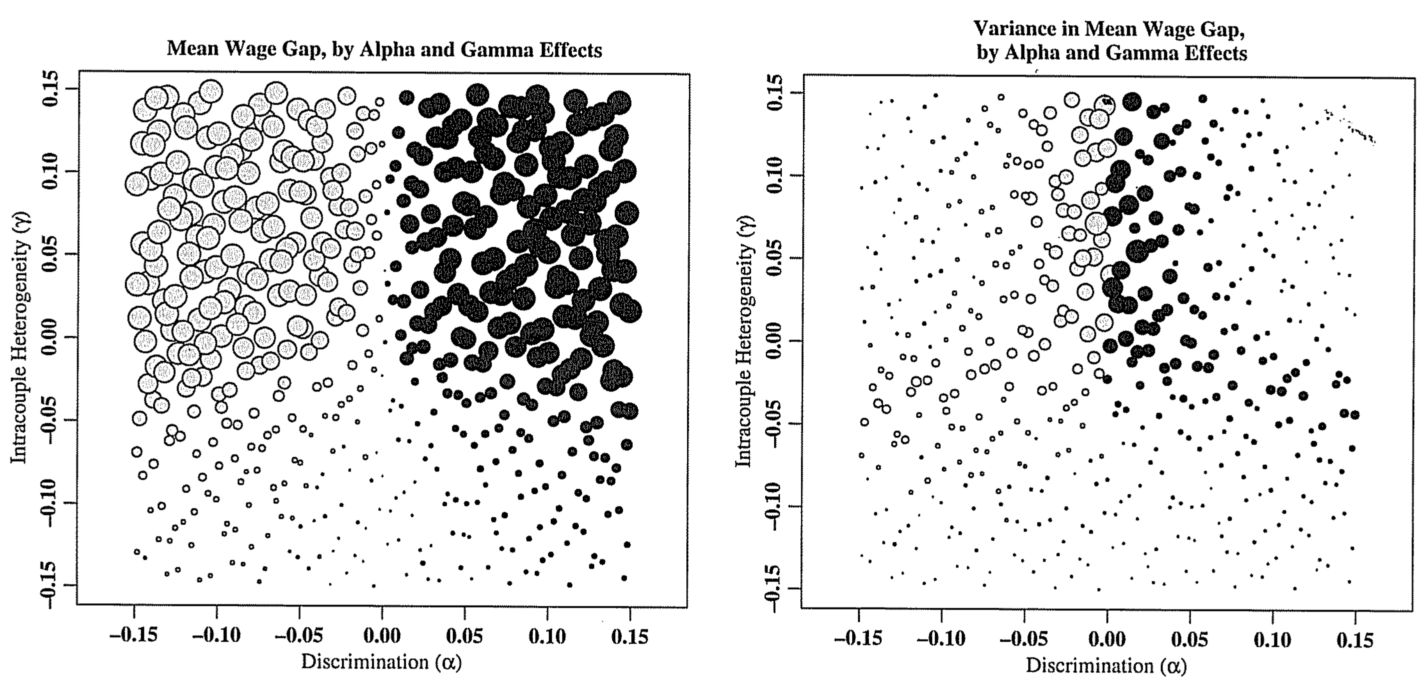


FIGURE 11.3. Gender difference in mean wage rank, discrimination, and couple-level homogeneity effects

the role of segregation is more complex. As the first panel of Fig. 11.2 shows, strong segregation effects substantially increase the rate of transition from one stratification regime (e.g., male dominant) to the other (e.g., female dominant); where segregation is strong, there is an almost immediate phase transition at $\alpha = 0$ from one regime to the other. A mixing regime (where the wage gap is of small magnitude) continues to exist near the origin, and enlarges slightly for $\beta > 0$. This confirms the intuition that supra-random mixing does inhibit convergence to a highly stratified regime, albeit weakly. The explanation for both effects lies in the way in which segregation effects alter the allocation of men and women to occupational categories. When segregation is strong ($\beta \ll 0$), each category tends to be occupied exclusively by members of a single gender; in the presence of even a weak discrimination effect, high-ranking categories will then tend to become the exclusive province of the dominant group, while the subordinated group will be similarly concentrated almost exclusively into the low-ranking blocks. By contrast, when $\beta \gg 0$, it becomes nearly impossible for any occupational category to be gender exclusive. Thus, there must be some members of the subordinate group in the high-ranking blocks, and some members of the dominant group in the low-ranking blocks. This makes extreme stratification much more difficult to achieve, hence the inhibitory effect on the wage gap. Interestingly, this same phenomenon implies a non-monotonic interaction with discrimination on the variance of the wage gap. When $\beta \ll 0$ and $\alpha \approx 0$, occupational categories are highly segregated with no general tendency for any particular category to be dominated by males or females. If, by chance, it happens that the males wind up with the high-end categories, then the wage gap will be large (and positive); these categories could be as easily dominated by females, however, in which case the gap will be negative but also of large magnitude. Thus, segregation in the absence of discrimination should act to greatly increase the variance of the wage gap, without impacting the mean. On the other hand, we have already seen that high segregation in the presence of discrimination results in a highly stratified regime, in which variance should be low. This divergence should disappear in the supra-random mixing case, since the net impact of this effect is to push the job allocation process toward uniformity. As it happens, we see all three of these phenomena in the second panel of Fig. 11.2, which shows the variance of the wage gap across the parameter space. Compared with the $\beta = 0$ baseline, $\beta \ll 0, \alpha \approx 0$ shows highly elevated variance, falling almost immediately to low levels as $\alpha$ increases in magnitude. By contrast, variance is much less sensitive to $\alpha$ where $\beta \gg 0$, tending to remain moderate even at more extreme $\alpha$ values.

Just as one can consider the effect of homogeneity or heterogeneity with respect to persons within the same occupation, one can also (via $\gamma$ effects) consider forces toward or away from heterogeneity with respect to couples. Mechanisms such as social influence (Freidkin 1998), homophily on unobserved characteristics (McPherson et al. 2001), and diffusion of opportunity for social ties (Calvo-Armengol and Jackson 2004) can potentially lead to a net tendency toward similarity of within-couple wage rates. By contrast, incentives for



specialization in home versus market production (Becker 1991), normative pressures for intensive parenting (Jones and Brayfield 1997), and the like can lead to high levels of intra-couple wage heterogeneity. To explore these effects, we replace the $\beta$ effect used to model segregation in Fig. 11.2 with a $\gamma$ effect for intra-couple wage heterogeneity, and simulate draws from the location system model. As shown in Fig. 11.3, the results are striking: while positive intra-couple heterogeneity effects slightly encourage convergence to a stratified regime, even modestly negative values dampen stratification altogether. How can this be? The secret lies in the observation that the absolute value of the male/female wage gap must be less than or equal to the mean of the absolute intra-couple wage differences. As a result, intra-couple wage heterogeneity acts as a "throttle" on the wage gap: force it to diminish (by setting $\gamma < 0$), and stratification must likewise decrease. This effect similarly reduces the variance of the wage gap (see Fig. 11.3, panel 2), resulting in a "homogeneous mixing regime" in which stratification is uniformly minimal. By contrast, high intra-couple heterogeneity requires one member of each couple to have a much higher wage rank than the other; like segregation, this inflates variance where discrimination is low, but reduces it where discrimination is high. Between, there exists a thin band of entropic mixing, where the various forces essentially cancel each other out.

While these simulations only hint at what is possible when using the location system to model occupational stratification, the effects they suggest are nevertheless interesting and non-obvious. Particularly striking is the relative power of couple-level heterogeneity effects in suppressing labor market discrimination, a result which suggests a stronger connection between processes such as mate selection and marital bargaining with macro-level stratification than might be supposed. The exacerbation of discrimination effects by discrimination is less surprising, but no less important, along with the somewhat weaker inhibiting effect of active desegregation. These phenomena highlight the importance of capturing dependencies among both individuals and among jobs when modeling stratification in labor market settings. Such effects can be readily parameterized using the location system, thereby facilitating a more complete theoretical and treatment of wage inequality within the occupational system.

### *11.5.2. Settlement Patterns and Residential Segregation*

Another problem of long-standing interest to social scientists in many fields has been the role of segregation within residential settlement processes (Schelling 1969; Bourne 1981; Massey and Denton 1992; Zhang 2004). Here, we illustrate the use of the location model on a stylized settlement system involving 1,000 households (objects) allocated to regions on a uniform 20-by-20 spatial grid (locations). Unlike the job allocation system described above, this system places no occupancy constraints on each cell; however, "soft" constraints may be implemented via density dependence effects. For purposes of demonstration, each household is assigned a random "income" (drawn independently from a log-normal distribution with parameters 10 and 1.5) and an "ethnicity" (drawn from two types, with 500 households belonging to each type). Households are tied to one another via social ties, here modeled simply as a Bernoulli graph with mean degree of 1.5. Regions, for their part, relate to one another via their spatial location. Here, we will make use of both Euclidean distances between regional centroids and Queen's contiguity (for purposes of segregation). Each region is also assigned a location on a "rent" gradient, which scales with the inverse square of centroid distance from the center of the grid.

With these building blocks, a number of mechanisms can be explored. Several examples of configurations resulting from such mechanisms are shown in Fig. 11.4. Each panel shows the 400 regions comprising the location set, with household positions indicated by circles. (Within-cell positions are jittered for clarity.) Household ethnicity is indicated by color, and network ties are shown via edges. While each configuration corresponds to a single draw from the location model, a burn-in sample of 100,000 draws was taken (and discarded) prior to

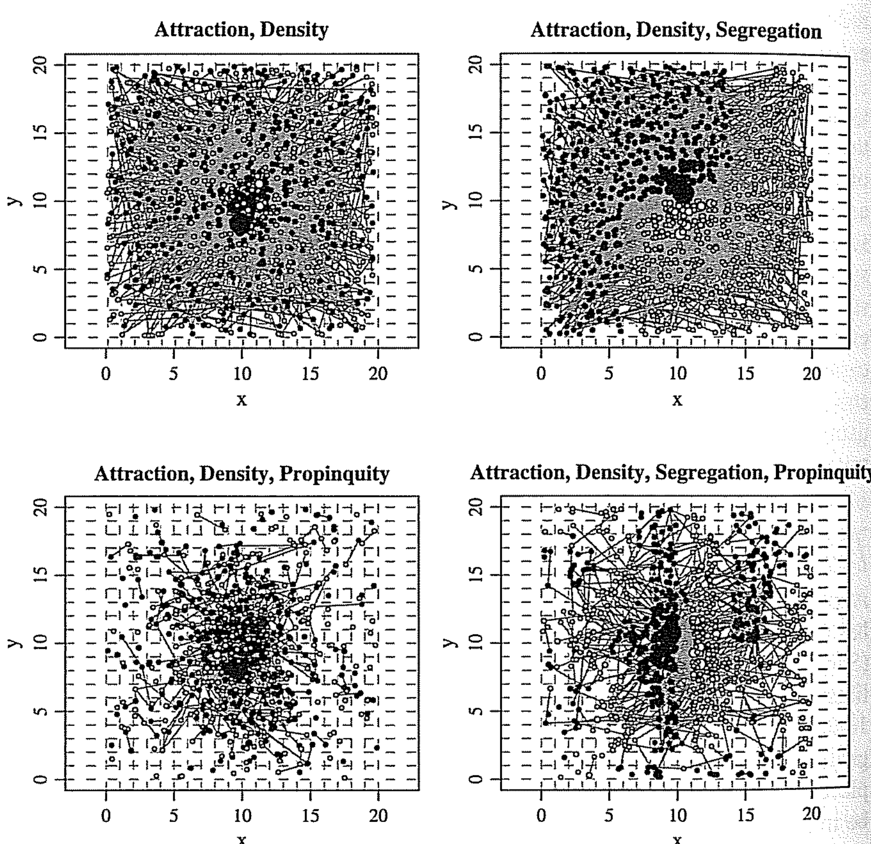


FIGURE 11.4. Location model draws, spatial model.



sampling. Configurations shown here are typical of model behavior for these covariates and parameter values.

The panels of Fig. 11.4 nicely illustrate a number of model behaviors. In the first (upper left) panel, a model has been fit with an attraction parameter based on an interaction between rent level and household income ($\alpha = 0.0001$), balanced by a negative density dependence parameter $\delta = -0.01$. (Density is modeled by an alignment statistic between an identity matrix (for locations) and a matrix of ones (for objects); the associated product moment is the sum of squared location occupancies.) Although the former effect tends to pull all households toward the center of the grid, the density avoidance effect tends to prevent "clumping." As a result, high-income households are preferentially clustered in high-rent areas, with lower-income households displaced to outlying areas. Note that without segregation or propinquity effects, neither ethnic nor social clustering are present; this would not be the case if ties were formed homophilously, and/or if ethnicity was correlated with income. Clustering can also be induced directly, of course, as is shown in the upper right panel of Fig. 11.4. Here, we have added an object homogeneity effect for ethnicity through Queen's contiguity of regions ($\beta = -0.5$), which tends to allocate households to regions so as to reduce local heterogeneity. As can be seen, this induces strong ethnic clustering within the location system; while high-income households are still preferentially attracted to high-rent areas, this sorting is not strong enough to overcome segregation effects. Another interesting feature of the resulting configurations is the nearly empty "buffer" territory which lies between ethnic clusters. These buffer regions arise as a side-effect of the contiguity rule, which tends to discourage direct contact between clusters. As this suggests, the neighborhood over which segregation effects operate can have a substantial impact on the nature of the clustering which results. This would seem to indicate an important direction for empirical research.

A rather different sort of clustering is generated by adding a propinquity effect to the original attraction and density model. Propinquity is here implemented as an alignment effect between the inter-household network and the Euclidean distance between household locations ($\delta = -1$). As one might anticipate, the primary effect of propinquity (shown in the lower-left panel of Fig. 11.4) is to pull members of the giant component together. Since many of these members also happen to be strongly attracted to high-rent regions, the net effect is greater population density in the area immediately surrounding the urban core. Another interesting effect, however, involves households on the periphery: since propinquity draws socially connected households into the core, peripheral households are disproportionately those with few ties and/or which belong to smaller components. The model thus predicts an association between social isolation and geographical isolation. Ironically, this situation is somewhat attenuated by the reintroduction of a residential segregation effect (lower-right panel). While there is still a tendency for social isolates to be forced into the geographical periphery, the consolidation of ethnic clusters limits this somewhat. Because ties are uncorrelated with ethnicity, propinquity also acts to break the settlement pattern into somewhat smaller, "band-like" clusters with interethnic ties spanning the inter-cluster buffer zones. (One would not expect to observe this effect in most empirical settings, however, due to the strong ethnic homophily of most social ties (McPherson et al. 2001).)

Broader information on the behavior of the settlement model can be obtained by simulating draws from across the parameter space, as with Figs. 11.1–11.3. (Simulations were performed in the same manner as those for the occupation model, but were thinned from 300,000 rather than 200,000 draws per chain.) Figure 11.5 shows the mean local heterogeneity statistic ($t^{\beta}$) for ethnicity by Queen's contiguity as a function of segregation ($\beta$) and propinquity ($\delta$) parameters. Each circle within the two panels reflects the mean or variance of the realized heterogeneity statistic (respectively), with circle shading indicating the corresponding mean or variance in the realized alignment statistic ($t^{\delta}$). As the figure indicates, a clear phase transition occurs at $\beta = 0$, as one transitions sharply from a segregated, low-variance regime to a heterogeneous, high-variance regime. Interestingly, the realized level of propinquity varies greatly only in the upper left-hand quadrant of the parameter space (an environment combining segregative tendencies with high $\delta$ values). Propinquity has no substantial effect on heterogeneity in this case, demonstrating that there exist some structural effects which are only weakly coupled.

Unlike propinquity, population density effects interact much more strongly with segregation. Figure 11.6 shows mean/variance in the realized population density (circle area) and heterogeneity (circle shading) statistics as a function of their associated parameters. Unsurprisingly, pressure toward density quickly tips the system into a highly concentrated population regime; somewhat more surprisingly, however, the variance of this state is much higher than the diffuse regime. This reflects the fact that pressures toward population density tend to lead to a rapid collapse into local clusters, which change only unevenly across draws: thus, there is rather more variability here in realized density than there is in the case where households are forced to spread thinly across the landscape. The low-density regime also tends to support high levels of homogeneity, while very high densities tend to inhibit it somewhat; interestingly, however, this inhibition appears to occur (in many parts of the parameter space) via a series of sudden phase transitions, rather than a gradual shift (the exception being the lower right-hand quadrant, in which heterogeneity pressure gradually overcomes resistance toward concentration). Thus, pressure toward or away from segregation can enhance or inhibit the concentration of population into small areas, and vice versa, and this process can occur very suddenly when on the border between regimes.

As Schelling long ago noted, even mild tendencies toward local segregation can result in residential segregation at larger scales (Schelling 1969). While the location system model certainly bears this out, the model also suggests that factors such as population density and inter-household ties can interact with segregation in non-trivial ways. Using the location system framework, such interactions are easy to examine, and the strength of the relevant parameters can

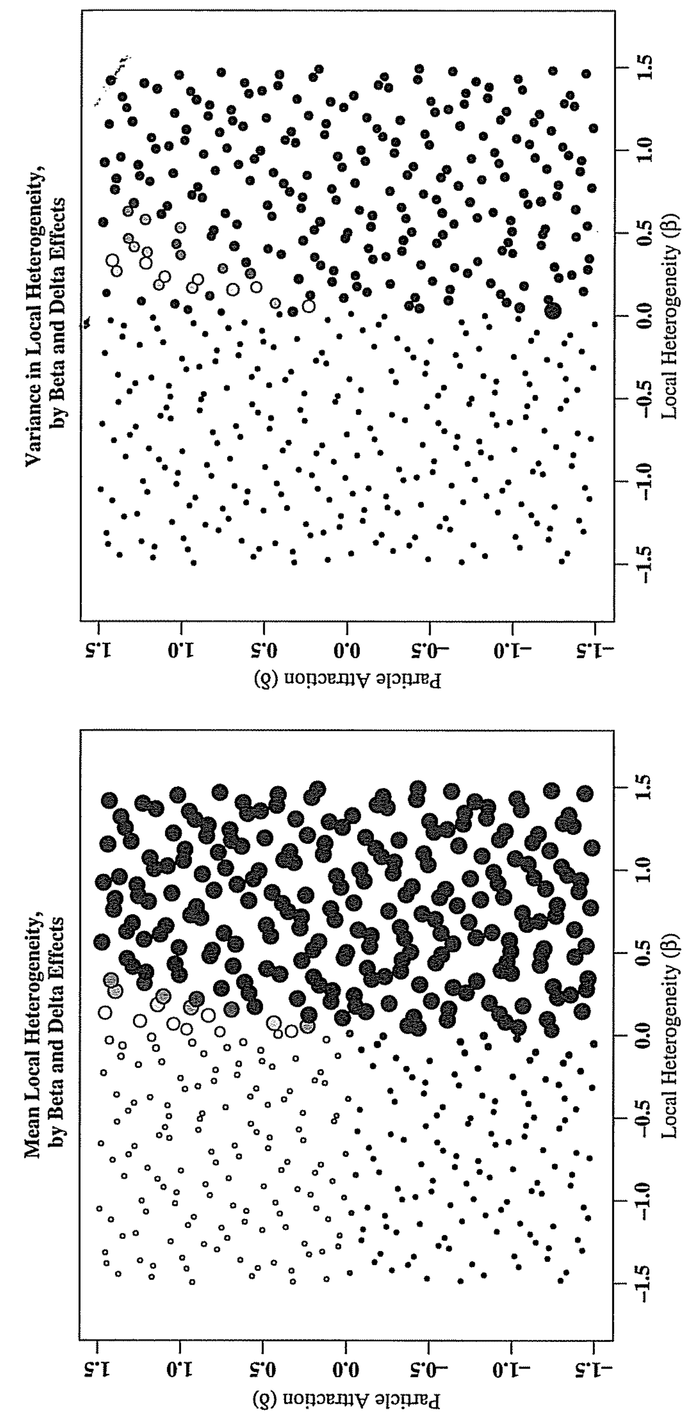


FIGURE 11.5. Mean segregation statistic, by segregation and propinquity effects

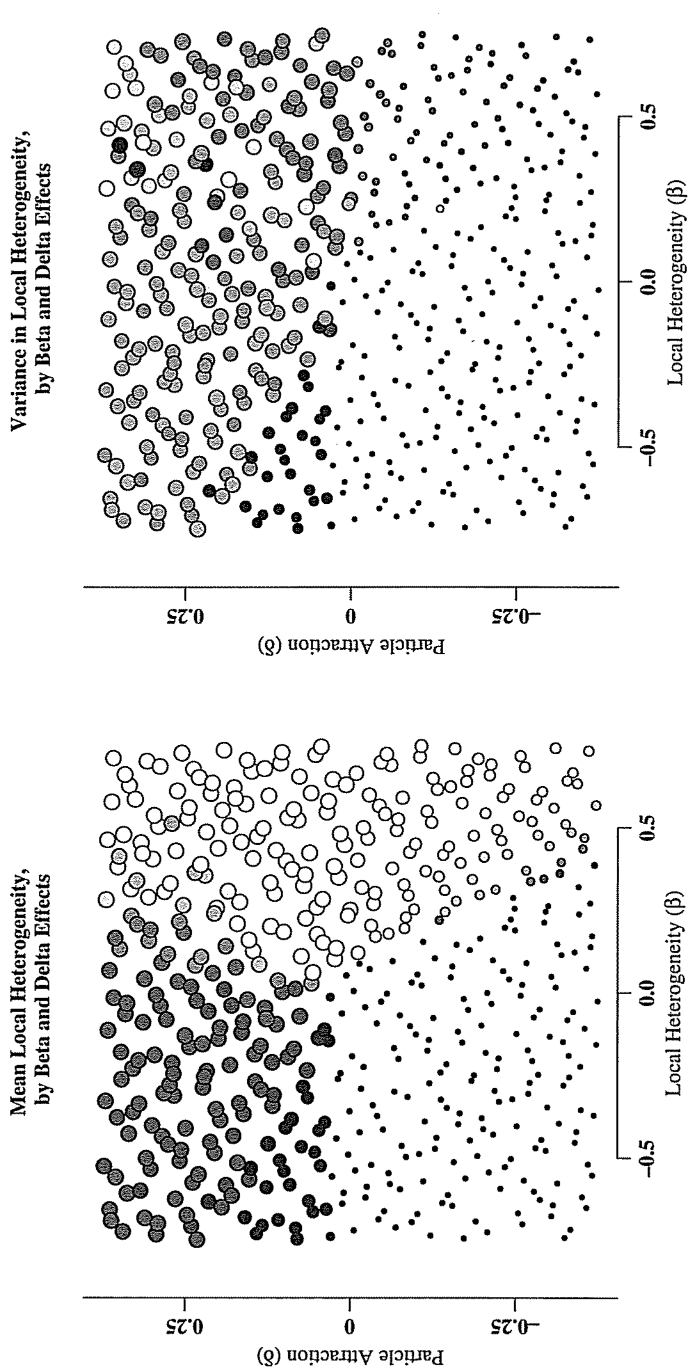


FIGURE 11.6. Mean concentration statistic, by density and segregation effects



be readily estimated from census or other data sources. It is also a simple matter to introduce objects of other types (e.g., firms) which relate to households and to each other in distinct ways (as represented through additional covariates). In an era in which geographical data is increasingly available, such capabilities create the opportunity for numerous lines of research.

## 11.6. Conclusions

In the foregoing, we have used a stochastic modeling framework (the generalized location system) to illustrate the applicability of physical models to a broad class of social systems. While the location system has antecedents in many fields (including spatial statistics and social networks), its strong formal connection with statistical mechanics is of particular relevance for researchers in areas such as constructal theory, who seek to identify productive ways of integrating physical principles into the social sciences. The applicability of the location system to problems such as occupational stratification and residential settlement patterns highlights not only the versatility of the model, but also the extent to which many apparently disparate social phenomena have strong underlying commonalities. Recognizing and exploiting those commonalities may allow us not only to cross-apply findings between the physical and social sciences, but also to leverage knowledge across different problems within the social sciences themselves.

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