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IOWARDS AN UNDERSIANDING OF MODELLING PROCESS

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ABSTRACT: *This paper considers the modelling of urban and transport systems and the methodology of model formulation. The use of reasoning by analogy is discussed, with an emphasis on the underlying mathematical concepts and principles, and the derivation of an individual choice model is given. The paper discusses the interpretation of land-use/transport systems models in terms of information theory and the theory of games, shedding light on the relevance of mathematical programming models to real world situations. The mathematical concepts also allow the model user to gain valuable insights into meaning, structure and solutions of particular models. A new urban planning model is used as an example.*

INTRODUCTION

The concepts behind the mathematical constructions in model building are often neglected in later interpretations of a particular model, and sometimes the worth and applicability of a model may be lost or disguised as a result. In urban and transport systems modelling the apparent dichotomy between macro-level and micro-level models might be lessened through a review of the mathematical foundations of some models. The understanding of particular models in practice might also be enhanced by stripping away the layers of equations to show the conceptual cores which lie beneath. This paper discusses the interpretation of an urban and transport planning model (OPUS, Optimal Planning of Urban Systems) in terms of information theory and the theory of games. It also describes the derivation of a behavioural choice model using a mathematical argument analogous to that used in quantum mechanics.

The paper thus allows for discussions of a number of important questions, such as possible relationships between macro-level (aggregate) and models of individual behaviour, and some insights on the relevance of mathematical programming planning models to real world situations. The theoretical concepts introduced may also permit the model user to better understand the meaning, structure and solutions of particular models without the need for the complexities of mathematical manipulations.

ANALOGIES IN MODELLING

The use of analogy in developing models of transport systems has had a chequered history. In the 1950s and 1960s many models were derived by analogies with the physical sciences (e.g. the gravity models of Voorhees (1955) and Wilson (1967), and the Boltzmann-like theory of traffic flow (Prigogine 1959)). In recent times modelling based on physical analogy has fallen into disfavour as theories based on individual behaviour have been developed (e.g. see Richardson and Young (1980) for discussion on the point). Human behaviour at the level of the individual would not seem to relate strongly to the behaviour of molecules in a gas. Further reflection on the matter of analogy can however lead to some useful principles. A model of a physical system may be seen as an application of a particular mathematical formulation. A set of concepts and assumptions yield mathematical equations which are then solved. The analogy does not come from the physical system itself, rather it stems from the mathematics. The particular systems analyzed are thus parallel examples of the application of a mathematical theory. In many cases the application to the physical system may have considerably predated the application to the human system. The question is thus not whether the two systems are analogous but rather if the assumptions underlying the mathematics are viable for each system, given constraints in terms of the available data, the results to be found, and the intended purposes of the results.

Consequently, the observation that a particular model structure first arose in another scientific field cannot be used as an argument for that model's acceptance or rejection. The only advantage of reasoning by analogy is that it may permit the analysis of certain phenomena in a consistent fashion according to a previously investigated logical system. Logical connections need not be assumed between sciences, rather full use can be made of any logical parallels existing between descriptive systems (Griesinger 1974). This idea is not new. James Maxwell (1890) argued that:

> 'By physical analogy, I mean that partial resemblance between the laws of a science and the laws of another science which makes one of the two sciences serve to illustrate the other.'

Two examples of modelling by physical analogy follow. The first describes the gravity model for trip distribution, and how its derivation has evolved from reasoning by direct physical analogy to the use of information theory. The second example outlines the generation of an individual choice model using the Schroedinger equation from quantum mechanics. This analogy produces a model similar to the multinomial logit model. Some of the underlying assumptions of the Schroedinger-derived model are then discussed.

The Gravity Model

The study of human spatial interactions using 'gravity models' has a considerable history. Carey (1858) suggested a 'great law of molecular gravitation', with the individual as the molecule of society, by direct analogy with physical gravitation. Subsequently Ravenstein (1885) offered empirical evidence to support such a model. The Boston Transportation Study of 1927 used an inverse-square-distance model to estimate trip interchanges between traffic zones (Heightchew 1979). This work was forgotten in the aftermath of the Great Depression and World War II, and the gravity model analogy for trip distribution was reformulated in the 1950s (Voorhees 1955). Subsequently Wilson (1967) derived the modern form of the gravity model using the concepts of statistical mechanics. It is now known that this derivation is in fact an application of the mathematical theory of information (Roy and Lesse 1981). Information theory offers a general mathematical framework for finding best estimates (most probable values) of specified model variables (or parameters) given the level of available data. It also indicates a system for refinement of estimated values as more data (information) are made available (e.g. Snickars and Weibull 1977). The approach thus offers a method of finding model outputs with a minimum of information and a means for improving these estimates as further information becomes available. It is the mathematics which produces the model rather than the analogy with the behaviour of particles in a physical system.

In information theory, entropy becomes the degree of uncertainty, related to the quantity of missing information. Recently Roy and Lesse (1981) described alternative microstate definitions which relate the possible orderings of individuals (e.g. trips, or households) into groups (e.g. zones) according to various constraints on group size (e.g. zone capacity) or variations between individuals. The particular definitions were shown to correspond to alternative definitions of entropy in physics, and to be simply described in terms of locational parameters in a transport systems context. The mathematical treatment of these concepts may be found in Snickars and Weibull (1977) and Roy and Lesse (1981), and the following results are known.

The common form of the (doubly-constrained) gravity model is

$$T_{ij} = A_i\, O_i\, B_j\, D_j \exp(\beta\, c_{ij}) \qquad (1)$$

where

$$A_i = 1/\sum_j D_j\, B_j \exp(\beta\, c_{ij}) \qquad \forall\, i$$

and

$$B_j = 1/\sum_i O_i\, A_i \exp(\beta\, c_{ij}) \qquad \forall\, j$$

given that T_{ij} is the number of trips between origin i and destination j, c_{ij} is the travel cost, O_i is the trip production and D_j is the trip attraction. Information theory permits the derivation of this model, given that the degree of uncertainty (entropy) of the system may be written as

$\sum_{ij} T_{ij} (\log T_{ij} - 1)$ (Katz 1967). The derivation follows from

solution of the mathematical programming problem

$$\max S = - \sum_{ij} T_{ij} (\log T_{ij} - 1) \qquad (2)$$

subject to

(a) a known total number of trips (T) $T = \sum_{ij} T_{ij}$ (3)

(b) origin-balance constraints $O_i = \sum_j T_{ij} \quad \forall\, i$ (4)

(c) destination-balance constraints $D_j = \sum_i T_{ij} \quad \forall\, j$ (5)

(d) mean cost of travel ($\bar{c}$) $T\bar{c} = \sum_{ij} T_{ij} c_{ij}$ (6)

Other common types of gravity model may be found by removing some of the constraints above. Singly-constrained models result from removing constraints (b) or (c) respectively. An unconstrained model yielding a trip distribution with the required mean travel cost results from the complete removal of constraints (b) or (c). Further models may be generated by adding extra constraints. For example if the variance (s^2) of the travel cost distribution is known then addition of the constraint

$$\sum_{ij} T_{ij} c_{ij}^2 = T(s^2 + \bar{c}^2) \quad (7)$$

would yield a model which balanced trip attractions and productions, and fitted the mean and variance of the travel cost distribution. Further constraints e.g. on subsets of origins and destinations or knowledge of higher moments of the cost distribution might also be used. These extra constraints represent increased levels of knowledge of the system under study. Eriksson (1980) has produced an efficient general computer program for solving maximum entropy problems of this type.

Field Theory and an Individual Choice Model

Field theory is a well-established branch of mathematical physics. Griesinger (1978) argued for a field theory in psychology based on the assumption that a psychological force (composed of values and perceptions at a decision time) could determine behavioural propensities. He sought both a relationship between the definition of utility and a choice rule, suggesting that the two concepts were interdependent, and a relationship between the functional form of the field and its sources.

Force is a vector, whereas utility in behavioural theory is a scalar. However, force is proportional to the gradient $\underline{\nabla}U$ of potential energy (U). Griesinger suggested that the definition of a generalized utility field might thus find inspiration from the study of the potential field in physics. Field souces in behavioural terms would be sources of expected satisfaction (Lewin 1938). The choice situation also requires possible extension to an abstract n-dimensional space (e.g. utility in terms of the value attributes of a commodity, as defined by Lancaster (1966) amongst others). A value of utility can then be defined for each point in the abstract space, and sources of utility may stem from actual experiences or judgements concerning some of the alternatives. Griesinger (1978) defined psychological force as the gradient of the scalar utility field, i.e.

$$\underline{F} = \underline{\nabla}U \quad (8)$$

An analogy with Newtonian physics did not yield a choice rule for decision theory (Griesinger 1978), whereas the Schroedinger equation from quantum mechanics could. The Schroedinger equation relates the potential energy field to the probability $P(r,t)$ of observing a particle in a volume element δv at a location r at time t, in terms of a probability amplitude $\Psi(r,t)$ and its complex conjugate $\Psi^*(r,t)$, and is given by

$$P(r,t) = \Psi^*(r,t)\ \Psi\ (r,t) \tag{9}$$

Consider the time-independent form of the Schroedinger equation which is (Irving and Mullineux (1959)

$$\nabla^2\Psi + m(U - \lambda)\ \Psi = 0 \tag{10}$$

where λ and m are constants, and the probability density function (preference function) $p(r)$ is

$$p(r) = \Psi^*\ (r)\ \Psi(r) \tag{11}$$

Equation (10) is a Sturm-Liouville equation whose solutions are known, and depend on the eigenvalue λ which in turn depends on the form of U and the boundary conditions (e.g. Irving and Mullineux 1959). These results are defined for a continuous space, while a choice situation is typically limited to a finite number of alternatives. A distinction is needed between the preference function and the choice probability (P_K, for alternative k) which is defined on a reduced space consisting solely of the perceived available alternatives (Luce 1959). In the present terminology, Luce's axiom gives the probability of choosing an alternative lying in a volume δv about the point r_i, given n alternatives lying in equal volume elements δv about the points r_i, $i = 1, \ldots, n$ as

$$P\ \{r_K\ |\ r_i,\ i=1,\ldots,\ n\} = p(r_K)/\sum_{i=1}^{n} p(r_i) \tag{12}$$

As an illustration of this reasoning, consider a point source at $r=0$ in an n-dimensional orthogonal Euclidean space with $U=a/r$ where a is a constant and r is the radial distance. Then, using the definition

$\nabla^2 r = \frac{\partial^2}{\partial r^2} + \frac{(n-1)}{r}\frac{\partial}{\partial r}$ for a radially-symmetric function in

this space, equation (10) may be written as

$$\frac{\partial^2\Psi}{\partial r^2} + \frac{(n-1)}{r}\frac{\partial\Psi}{\partial r} + m(\frac{a}{r} - \lambda)\ \Psi = 0 \tag{13}$$

which is a well-known equation whose solution for λ_o (the first eigenvalue, or groundstate) is

$$\lambda_o = a^2 m/(n-1)^2 \tag{14}$$

$$\Psi_0 = L \exp(-amr/(n-1))$$

so that, substituting in equation (11)

$$p = L^2 \exp(-2amr/(n-1)) \quad (15)$$

where L is a constant. From equation (12) it follows that

$$P(r_k) = \exp(-am\ r_k)/ \sum_i \exp(-am\ r_i) \quad (16)$$

which is a similar form to the multinomial logit choice model.

The selection of alternative definitions of the utility function would result in alternative forms of the choice model. Griesinger (1978) used this method to model a number of well-known psychological phenomena. A critical review of this procedure is required, however. In the first instance the definition of the attribute space needs to be carefully considered. The assumption of orthogonality is important, representing an attribute-set free of multi-collinearity. The choice of a Euclidean space may also restrict the selection and application of a utility function. More importantly, the derivation of equation (10) involves an assumption that the behaviour of the individual is periodic in time, and is confined within certain fixed bounds. Such a situation might well exist for some choice situations (e.g. the journey to work) but the validity of a model such as that given in equation (16) needs to be carefully examined in any intended application. Despite these criticisms Griesinger's methodology offers an area of considerable interest for future research.

This section discussed the general use of analogy in systems modelling, and indicated that the use of a particular model structure in one scientific field should not be used per se as an argument for acceptance or rejection of that structure in another field. Rather the consideration of the usefulness of a model needs to be based firstly on the applicability and restrictions of the assumptions behind the model, and subsequently on the data requirements and desired level of model output.

In the next section an alternative methodology for the interpretation of models is addressed. As an example, a new general urban systems model is examined, using the theory of games, to relate and compare alternative model structures.

A NEW URBAN SYSTEMS MODEL

Recent work at CSIRO Division of Building Research has centred on the development of a new combined land-use/transport planning model (OPUS), which includes transport costs, and the costs of land-use development and the demolition of existing land-use activities (i.e. urban growth, redevelopment and/or decline). The OPUS model may be seen as a multiple objective comparative planning model, and includes the earlier TOPAZ model (Sharpe and Brotchie 1972, Sharpe and Karlqvist 1980, Brotchie, Dickey and Sharpe 1980) as one component. Other components, involving alternative objective functions, are planned, and the first of these to be implemented is a model generating a (co-operative or optimum) lower bound solution for the combined land-use/transport problem which permits trade-offs between efficient transport costs (e.g. energy) and land-use cost alternatives to be evaluated. The model formulation is given in the Appendix to this paper. It will be seen later that TOPAZ may be interpreted as a competitive or 'Nash' gaming model whereas the co-operative model is a 'Pareto' gaming model.

The main point of interest here is the interpretation of the OPUS model and comparisons between its component sub-models. The mathematical theory of games offers a useful method of interpretation, which may have application to a wide range of mathematical programming models. A brief outline of this theory follows.

Theory of Games

The clearest interpretation of the theory of games may be seen for the case of two players, each of whom tries to optimize his own objective function (U_1 for player 1, U_2 for player 2) in terms of two control variables (x_1 and x_2). The results may easily be extended to n players and m control variables (e.g. see Von Neumann and Morgenstern 1953). In the case of two players and two control variables, a useful geometric interpretation of the problem may be used as in Figure 1. Player 1 tries to select his control variable x_1 to minimize his pay-off U_1 while player 2 tries to select his control variable x_2 to minimize his pay-off U_2. O_1 and O_2 in Figure 1 represent the global minima for U_1 and U_2 respectively, and the contours represent the form of the two functions U_1 and U_2. The dashed lines passing through O_1 and O_2 represent the loci of rational (optimizing) choices for Players 1 and 2 for fixed values of x_2 and x_1 respectively. The point(s) of intersection (if any) of these 2 loci represent solutions of the joint optimization problem in a competitive game. Point N on Figure 1 is such a point, and is called the 'Nash equilibrium'. If more than one such point exists, the player who has first move has the opportunity to select the Nash equilibrium point most favourable to him. At $N = (x_1^*, x_2^*)$, the following relations hold

$$\begin{aligned} & U_1(x_1^*, x_2^*) \leq U_1(x_1, x_2^*) \\ \text{and} \quad & U_2(x_1^*, x_2^*) \leq U_2(x_1^*, x_2) \end{aligned} \qquad (17)$$

In this situation no player can deviate unilaterally from N without worsening his own pay-off.

The shaded region S of Figure 1 represents an area in which both players can simultaneously improve their pay-off from the Nash equilibrium. However to achieve any such improvement, both players must agree to co-operate in the choices of their respective control variables. The concept of Pareto-optimal (non-inferior) solutions may be introduced to eliminate many of the solutions from region S in the search for the best solution in a co-operative game. The line O_1APBO_2 representing the loci of tangent points between the contours of U_1 and U_2 can be shown to have the property that every point on the line is not dominated by any other point Q in its neighbourhood (Rao and Hati 1980), i.e.

$$U_1 (P) \leq U_1 (Q) \quad \text{and} \quad U_2 (P) \leq U_2 (Q) \tag{18}$$

where P is a point on O_1APBO_2 and Q is any other point in S. The set of all points P on the line segment APB is the Pareto-optimal set, termed S_p. The set S_p may be determined from the following minimization set

$$Z(x, \alpha) = \alpha_1 U_1 (x_1, x_2) + \alpha_2 U_2 (x_1, x_2)$$
$$Y (\alpha) = \min_x [Z(x, \alpha)] \tag{19}$$

where $\alpha_1 + \alpha_2 = 1$; $\alpha_1 \geq 0$, $x=(x_1, x_2)$ and $\alpha = (\alpha_1, \alpha_2)$. If for a given α, x^0 minimizes $Z (x, \alpha)$ then a typical element of S_p may be written as

$$U(x^0) = \{U_1 (x_1^0, x_2^0), U_2 (x_1^0, x_2^0)\}$$

as S_p is the set

$$S_p = \{U(x^0) \mid x^0 \text{ minimizes } Z(x, \alpha)\} \tag{20}$$

which may be determined by solving a series of scalar minimization problems with x_1 and x_2 'co-ordinated by an umpire' (Rao and Hati 1980). The selection of the Pareto optimum then becomes a matter of finding the value of α maximizing Z in equation (19). The Pareto optimum $Y(\alpha = 0.5)$ is the most democratic one if no favour is to be shown to either player.

OPUS Submodels

The OPUS planning model may be seen as a comparative model which permits the analysis of land-use transport plans under a number of different criteria which can be related through gaming theory. The TOPAZ submodel (Brotchie, Dickey and Sharpe 1980) may be seen as a competitive game involving two players with one player sub-optimizing the land-use problem while the other sub-optimizes the transport distribution problem. The first player may be visualized as the planning authority, while the latter may be seen as the travelling public acting as a group. In this competitive game each player sequentially makes optimizing decisions according to the last move of the other player, and a Nash equilibrium solution emerges (Roy and Lesse 1981, personal communication). No direct co-operation between players occurs, and hence the final solution is not expected to be as good as one in which the players make simultaneous decisions.

If the players co-operate to jointly optimize land use and trip distribution then the solution is the Pareto optimum described earlier. Sharpe (1981, unpublished notes) solved this problem using Benders' decomposition technique, which allows the transport sub-problem to signal to the land-use master problem the effect of land-use changes on total transport costs, through the use of marginal cost (dual) variables. The master problem is then constrained to move towards the Pareto optimum by the generation of additional constraints (termed Benders cuts). The description of the mathematical programming problem representing the co-operative game is shown in the Appendix.

The Pareto optimum solution represents a lower bound solution for the land-use transport problem, and together with the Nash equilibrium solution can provide planners with more balanced information about the merit of alternative plans (Roy, Sharpe and Batten 1981). In line with a central theme of this paper it should be noted that linear programming (LP) techniques are used extensively in the solutions of the OPUS submodels. The submodels are not simply LP models, restricted to strict cost minimization and the treatment of land-use and trip distribution variables as simple homogeneous quantities, impervious to diversity of behaviour and perception. Rather the LP technique is used solely for the solution of parts of more complex problems which do permit variations in individual behaviour and allow for differing objectives to be held by competing groups.

CONCLUSIONS

The paper discussed the interpretation of a set of urban and transport planning system models in terms of the mathematical concepts underlying the models, with particular emphasis on the theory of games and information theory. The applicability of particular model forms was discussed in terms of their assumptions and resulting mathematical structures, with an indication that the use of similar model structures in other fields of science did not necessarily add to or decrease the relevance of a given model. An understanding of the underlying mathematical concepts behind a model can lead to an improved appreciation of the value and relevance of a model in particular circumstances.

In the final assessment, the real test of any model is the extent to which it can use known data and provide adequate and competent estimates on the basis of that data. Model testing and evaluation remains an important area for future study and research. Ultimately it is a model's relationship to data which will determine its significance.

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APPENDIX: AN OPTIMUM ECONOMIC/ENERGY LAND-USE TRANSPORTATION MODEL

This appendix develops a model to minimize the total combined energy (or cost) of transport, land-use development and demolition of existing activity, and which yields a lower-bound (Pareto) optimum solution, as a submodel within the OPUS urban planning model system outlined in the body of this paper. The objective is to determine a land-use and trip distribution pattern to:
(a) maximize the total benefits less costs of interaction plus,
(b) the total benefits less costs of establishing and operating land-use activities plus
(c) the total benefits less costs of demolishing or removing any development from an earlier period. Benefits and costs may be in either economic or energy units. The allocation is made subject to constraints requiring each activity to be fully allocated and that each zone is not overfilled. Additional planning and transport systems constraints may also be included.

Assume the following notation:

A_i = planned level of activity i including existing development.

b_{ij} = unit cost less benefit of incrementing the level of activity i in zone j.

$c_{ijk\iota}$ = cost less benefit per unit of interaction between activity i in zone j and activity k in zone ι.

d_{ij} = unit cost less benefit of decrementing the level of activity i in zone j.

e_{ij} = initial level of activity i existing in zone j.

s_{ik} = trip generation rate between a unit of activity i and a unit of activity k.

r_{ik} = $s_{ik} A_i/A_k$.

$T_{ijk\iota}$ = number of trips between activity i in zone j and activity k in zone ι.

x_{ij} = amount of activity i allocated to zone j.

y_{ij} = amount of activity i removed from zone j.

z_j = capacity of zone j, including existing development.

On the basis of a gravity model trip distribution with exponential deterrence function parameters $\{\beta_{ik}\}$ for trips between activities i and k, the overall problem may be written as

$$Z = \text{Min}_{T,x,y}[\textstyle\sum_{ijk\ell} (T_{ijk\ell}\, c_{ijk\ell} + T_{ijk\ell}\,(\log T_{ijk\ell} - 1)/\beta_{ik}) + \sum_{ij} (b_{ij}\, x_{ij} + d_{ij}\, y_{ij})] \tag{21}$$

subject to (i) interaction origin-destination constraints,

$$\textstyle\sum_{\ell} [T_{ijk\ell} - s_{ik}\,(x_{ij} - y_{ij} + e_{ij})] = 0 \quad \forall \quad i,j,k \tag{22}$$

$$\textstyle\sum_{j} [T_{ijk\ell} - r_{ik}\,(x_{k\ell} - y_{k\ell} + e_{k\ell}] = 0 \quad \forall \quad i,k,\ell \tag{23}$$

(ii) full allocation of each activity,

$$\textstyle\sum_{j} (x_{ij} - y_{ij}) = A_i - \sum_j e_{ij} \quad \forall \quad i \tag{24}$$

(iii) no zone overfilled,

$$\textstyle\sum_{i} (x_{ij} - y_{ij}) \leq Z_j - \sum_i e_{ij} \quad \forall \quad j \tag{25}$$

(iv) and constraint bounds

$$0 \leq (x_{ij})_{min} \leq x_{ij} \leq (x_{ij})_{max} \quad \forall \quad i,j \tag{26}$$

$$0 \leq (y_{ij})_{min} \leq y_{ij} \leq (y_{ij})_{max} \leq e_{ij} \quad \forall i,j \tag{27}$$

$$0 \leq (T_{ijk\ell})_{min} \leq T_{ijk\ell} \leq (T_{ijk\ell})_{max} \quad \forall i,j,k,\ell \tag{28}$$

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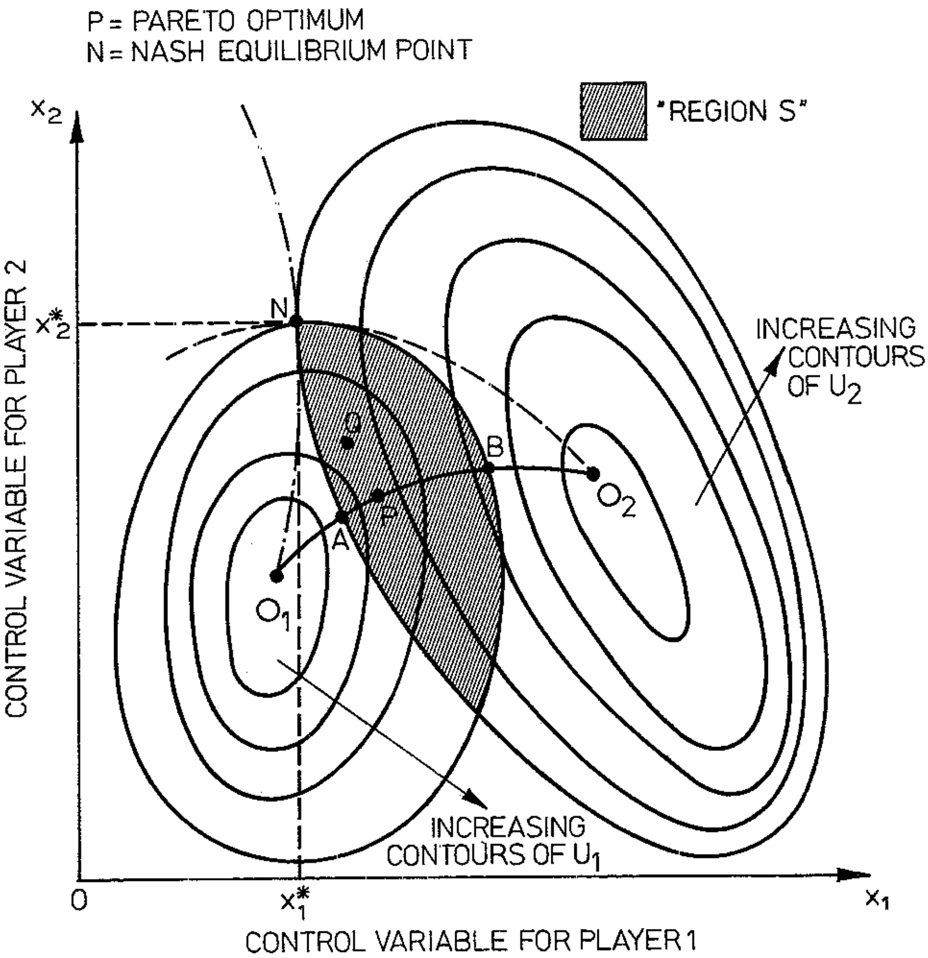

Figure 1. Graphical representation of the two-player game.