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SIMULATION AND MODELLING

CONTINUOUS TIME STOCHASTIC COMPARTMENTAL MODELS OF DISCRETE POPULATIONS

Richard L. Patterson

School of Natural Resources, University of Michigan

PRELIMINARIES

Let $[X(t);t>0]$ denote continuous time, n-state semi-Markov process with stochastic transition matrix $P=(p_{ij})$, state residence time distribution function matrix $W=[w_{ij}(z)]$, and stochastic interval transition probability matrix $F=[f_{ij}(t)]$ $(i, j=1,\dots,n)$. $X(t)$ is the state of the process at its most recent change of state and element $f_{ij}(t)$ of F is the conditional probability that $X(t)=j$ at time t, given that the initial state $X(0+)$ is i. Elements of F are related to elements of P and W by a Markov renewal equation of the Volterra type whose solution can be expressed by conditioning on the number of changes of state of the process prior to time t:

$$f_{ij}(t)=\sum_{\ell=0}^{\infty}\Pr[X(t)=j/X(0+)=i,1 \text{ changes of state in } (0,t)]\times \Pr[1 \text{ changes of state in } (0,t)/X(0+)=i] =$$

$$\delta_{ij}\cdot h_i(t)+p_{ij}\int_0^t w'_{ij}(z)\cdot h_j(t-z)\,dz+ \sum_{\ell=2}^{\infty}\Big[\sum_{q_1=1}^{m}p_{iq_1}\sum_{q_2=1}^{m}p_{q_1q_2}\cdots\sum_{q_{k-2}=1}^{n}p_{q_{k-3}q_{k-2}}\sum_{q_k=1}^{n}p_{q_{k-2}q_{k-1}}\cdot p_{q_{k-1}q_1}\times$$

$$\times\Big[\int_0^t(w_{iq_1}*w_{q_1q_2}*\dots*w_{q_{k-2}q_{k-1}}*w_{q_{k-1}q_1})'(z)\cdot h_j(t-z)\,dz\Big]$$

$$(i,\ j=1,\dots,n) \quad \text{(eqn. 1)}$$

where:

$q_1=j$;

$\int_0^t(w_{iq_1}*\dots*w_{q_{k-1}q_1})'(z)\cdot h_j(t-z)\,dz$,

an 1-fold convolution density convolved with $h_j(t)$, is multiplied by the probability $(p_{iq_1}\cdot\ldots\cdot p_{q_{k-1}q_1})$ that the 1-step sequence of changes of state $(i,q_1:\dots;q_{k-1},q_1=j)$ occurs:

$h_i(t)=1-\sum_{k=1}^{m}p_{ik}\cdot w_{ik}(t)$;

state j is assumed to be reachable from state i so that there is at least one 1-step sequence with positive probability.

When P is upper or lower diagonal the infinite sum on the right hand side of eqn. (1) terminates for $1>n+1$.

Let C denote a discrete population in which the behavioral states of individuals are in one-to-one correspondence with the states of $[X(t)]$. Let $S=(P,W,F)$ denote the system governing movement of individuals among behavioral states once they enter S from external sources. The conditional probability that an individual is in state j at time $t>0$, given that it initially entered S at time z $(0<z<t)$ in state i is $f_{ij}(t-z)$. Once inside S individuals are assumed to behave independently unless otherwise specified.

Subsets of states, aggregated into K non-overlapping and exhaustive subsets $G_1,\dots,G_K$ are called compartments $(K=2,\dots,n-1)$. The probability $f_{iG_k}(t-z)$ that an individual entering state i at time $z>0$ is in compartment G_k at time $t>z$ is:

$$f_{iG_k}(t-z) = \sum_{\text{state } j \text{ in } G_k} f_{ij}(t-z) \quad \text{(eqn. 2)}$$

Let $Y_{ij}(t)$ $(i,j=1,\dots,n)$ be random variables denoting numbers of individuals in states $1,\dots n$ at time $t>0$ whose initial entry into S is through state i.
The number $Y_{iG_k}(t)$ of individuals in compartment G_k at time t is:

$$Y_{iG_K}(t) = \sum_{\substack{\text{state } j\\ \text{in } G_k}} Y_{ij}(t) \qquad \text{(eqn. 3)}$$

The mean and variance of $Y_{iG_K}(t)$ is determined for different assumptions about processes of arrivals to S from external sources.

INDIVIDUAL POISSON ARRIVALS

Assume a Poisson stream of individual arrivals to S. Given that N_i arrivals occur in (0,t) to initial state i the joint p.f. of numbers in states 1,...,n at time t is multinomial with parameters $N_i, f_{i1}(t),\ldots,f_{in}(t)$. Multiplying the joint p.f. by the Poisson probability of N_i arrivals in (0,t) conditional on the arrival times of the first N_i arrivals being distributed as the order statistics of N_i independent samples from the d.f. on (0,t) having density $\lambda_i(z)/\int_0^t \lambda_i(z)\,dz$ $(0<z<t)$ the resulting joint p.f. is a product of n independent Poisson probabilities that $y_{i1},\ldots,y_{in}$ individuals are in states 1,...,n at time t:

$$P[Y_{i1}(t)=y_{i1},\ldots,Y_{in}(t)=y_{in}, N_i \text{ arrivals}] = \prod_{j=1}^{m} \frac{(\lambda_i(z).f_{ij}(t-z)dz)^{y_{ij}}}{y_{ij}!} \cdot e^{-\int_0^t \lambda_i(z).f_{ij}(t-z)dz} \qquad \text{(eqn. 4)}$$

$$(y_{i1}+\ldots+y_{in}=N_i)$$

As shown by eqn. (4) the $Y_{ij}(t)$'s are mutually independent Poisson distributed r.v.'s Moreover:

i) the arrival stream to state j is Poisson distributed with intensity $a_j(t)$ which satisfies the integral equation:

$$\int_0^t a_j(z).\sum_{k=1}^{m} p_{jk}.[1-w_{jk}(t-z)]dz = \int_0^t \lambda_i(z).f_{ij}(t-z)dz; \quad (j=1,\ldots n)$$

ii) the expectation of $Y_{ij}(t)$ is:

$$E[Y_{ij}(t)] = \int_0^t \lambda_i(z).f_{ij}(t-z)dz \qquad \text{eqn. (5)}$$
$$(j=1,\ldots n)$$

Equations (5) when combined with equations (1) provide the basis for constructing families of regression models of inputs to the system S as well as inputs and outputs among states within S, from which parameters can be estimated. Maximum likelihood estimates of parameters can be obtained from eqn. (4).

The r.v.'s $Y_{iG_k}(t)$ are independent and Poisson distributed with Poisson arrival intensities $a_{iG_k}(t)$ and expectations:

$$E[Y_{iG_k}(t)] = \int_0^t \lambda_i(z).f_{iG_k}(t-z)dz =$$

$$= \int_0^t \lambda_i(z).dz. \sum_{\substack{\text{state } j\\ \text{in } G_k}} f_{ij}(t-z) \qquad \text{eqn. (6)}$$
$$(k=1,\ldots K)$$

BATCH POISSON ARRIVALS

Individuals arrive at initial state i in batches, at random (Poisson arrivals) where the mean and variance of the i.i.d. batch sizes are m_i and v_i respectively. The intensity of arrivals is $\lambda_i(t)$. The marginal d.f. of $Y_{ij}(t)$ in this case is not Poisson unless $v_i=0$ and $m_i=1$. The mean and variance of $Y_{ij}(t)$ are:

$$E[Y_{ij}(t)] = m_i.\int_0^t \lambda_i(z).f_{ij}(t-z)dz$$
$$(j=1,\ldots,n) \qquad \text{eqn. (7)}$$

and:

$$\mathrm{Var}[Y_{ij}(t)] = m_i .\int_0^t \lambda_i(z).f_{ij}(t-z).[1-f_{ij}(t-z)]dz +$$

$$+ (m_i^2+v_i) . \int_0^t \lambda_i(z).[f_{ij}(t-z)]^2 dz +$$

$$+ v_i . [\int_0^t \lambda_i(z).f_{ij}(t-z)dz]^2 \qquad \text{eqn. (8)}$$
$$(j=1,\ldots n)$$

Equation (8) is demonstrated by first decomposing $Y_{ij}(t)$ into the random sum of "clusters" of sizes 1,2,...,B:

$$Y_{ij}(t) = 1.D_{i1}(t) + 2.D_{i2}(t)+\ldots+B.D_{iB}(t) \qquad \text{eqn. (9)}$$

where:

$D_{ik}(t)$ is a Poisson distributed r.v. with expectation:

$$E[D_{ik}(t)] = \int_0^t \lambda_i(z)\cdot\binom{B}{k}\cdot [f_{ij}(t-z)]^k \cdot dz \cdot [1-f_{ij}(t-z)]^{B-k} \quad (k=1,2,\ldots,B)$$

For a batch of given size B arriving at initial state i at time z a cluster of k-out-of-B of the arriving individuals will be in state j (t-z) time units later with binomial probability:

$$\binom{B}{j}\cdot [f_{ij}(t-z)]^k \cdot [1-f_{ij}(t-z)]^{B-k}$$

Combining the relation:

$$Var[Y_{ij}(t)] = E[Var(Y_{ij}(t)/B)] + Var[E(Y_{ij}(t)/B)]$$

with eqn.(9), eqn (8) is obtained. The distribution of the number of clusters in state j at time t without regard to the cluster size for fixed size B of arriving batches is Poisson distributed with expectation:

$$\int_0^t \lambda_i(z)\,.dz.\sum_{r=1}^{B}\binom{B}{r}.[f_{ij}(t-z)^r.[1-f_{ij}(t-z)]^{B-r}$$

Members of a given cluster have not necessarily been in residence in state j for the same length of time, however.

The mean and variance of the number of individuals in compartment G_k at time t are obtained by substituting $f_{iG_k}(t-z)$ for $f_{ij}(t-z)$ in equations 7 and 8.

ARBITRARY BUT FIXED INTERVALS BETWEEN ARRIVALS OF BATCHES

Batches of individuals, where batch sizes are i.i.d. random variables with mean m_i and variance v_i arrive at initial state i at arbitrary but fixed times $t_1, t_2, \ldots$ For a batch arriving at time t_u and of conditional size B_u the joint p.f. of numbers in states $1,2,\ldots,n$ at time $t > t_u$ is multinomial with parameters $B_u, f_{i1}(t-t_u), \ldots, f_{in}(t-t_u)$.

The marginal p.f. of the number $Y_{ij}(t)$ of individuals in state j at time t due only to the arriving batch at initial state i at time t_u of random size B_u has a compound form with mean and variance:

$$E[Y_{ij}(t)/t_u] = m_i \cdot f_{ij}(t-t_u) \qquad \text{eqn.}(10)$$

and:

$$Var[Y_{ij}(t)/t_u] = m_i \cdot f_{ij}(t-t_u)\cdot[1-f_{ij}(t-t_u)] + v_i \cdot [f_{ij}(t-t_u)]^2 \qquad \text{eqn.}(11)$$

If batch size is a fixed constant m_i then equation 11 is modified by setting v_i equal to zero.

The mean and variance of $Y_{iG_k}(t)$ are obtained by substituting $f_{iG_K}(t-z)$ for $f_{ij}(t-z)$ into equations 10 and 11.

The mean and variance of the marginal d.f. of the number of individuals in compartment G_k due to all arriving batches at times $0<t_1,\ldots,t_u<t$ is, assuming independence of all movements of individuals entering upon S:

$$E[Y_{iG_k}(t)/t_1,\ldots,t_u] = \sum_{r=1}^{u} E[Y_{iG_k}(t)/t_r] \quad (k=1,\ldots,K) \qquad \text{eqn.}(12)$$

and:

$$Var[Y_{iG_k}(t)/t_1,\ldots,t_u] = \sum_{r=1}^{u} Var[Y_{iG_k}(t)/t_r] \quad (k=1,\ldots,K) \qquad \text{eqn.}(13)$$

As with equations 5, equations 6, 7, and 12 can be used as the basis of constructing regression estimates of parameters of the system S.

SUB AND SUPER SYSTEMS OF S

The system S=(P,W,F) may be decomposable into subsystems $S_1,\ldots,S_K$ identified with compartments $G_1,\ldots,G_K$ or it may itself be a subsystem of a larger supersystem of states in which S is identified with a compartment G_S. In either case it is important to maintain stochasticity of the state transition matrices and the interval transition matrices corresponding to each subcollection of states that are to be identified with a subsystem.

Let $G_1,\ldots,G_K$ denote a collection of compartments of S and arrange the transition matrix P into the form:

$$P = (P_{G_iG_j}) \quad (i,j = 1,2,\ldots,K)$$

where:

the submatrix $P_{G_iG_j}$ has row and column dimension equal, respectively, to the number of states in compartments G_i and G_j.

Main diagonal submatrices contain state transition probabilities governing movements of individuals among states within compartment $(G_i(i=1,\ldots,K)$. Either advance or return to states in G_j from states in G_i is restricted by the number and locations of positive entries in off-diagonal submatrices $P_{G_iG_j}$. If no positive entries occur in $P_{G_iG_j}$ for all indices i and j then the system S consists of K independent subsystems. Each submatrix $P_{G_iG_j}$ is stochastic as well as the submatrix $F_{G_iG_i}$ of interval transition probabilities describing the time rate of movement of individuals among states of compartment G_i. Equations 1-13 are valid for each subsystem $S_1,\ldots,S_K$ in this case.

If compartments G_i and G_j are linked by positive entries in off-diagonal submatrix $P_{G_iG_j}$ then submatrix $P_{G_iG_i}$ is not stochastic and movements of individuals within compartment G_i cannot be analyzed independent of other states of S. By joining G_i to one additional absorbing state accounting for movements of individuals out of G_i and assigning transition probabilities into the appended absorbing state equal to one minus the row sums $P_{G_iG_i}$ for each row in the submatrix, the compartment G_i can be analyzed in either one of two ways:

i) as a subsystem in which arrivals are from other states of S or
ii) as a subsystem in which arrivals are assumed to occur without reference to prior movements in S.

If the system S is composed of states which are themselves a compartment of a supersystem, then S functions independently of other compartments or else S contains an absorbing state as described above so that movements of individuals within S can be analyzed independently of their movements within other compartments.