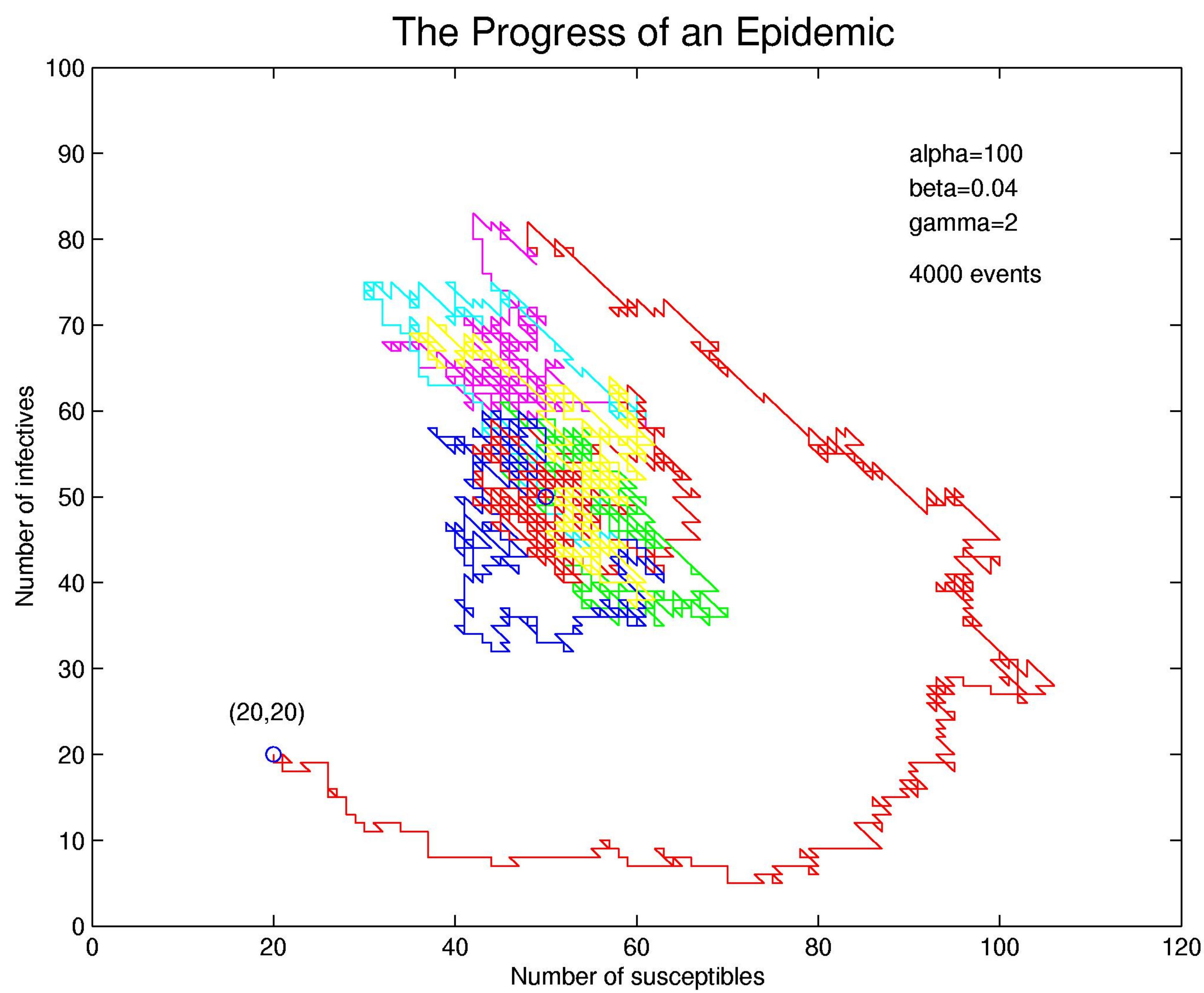

The Progress of an Epidemic
alpha=100
beta=0.04
gamma=2
4000 events
(20,20)
Number of infectives
Number of susceptibles
0
10
20
30
40
50
60
70
80
90
100
0
20
40
60
80
100
120

AN EPIDEMIC MODEL

The state at time t:

$X(t)$ - number of susceptibles

$Y(t)$ - number of infectives

State space:

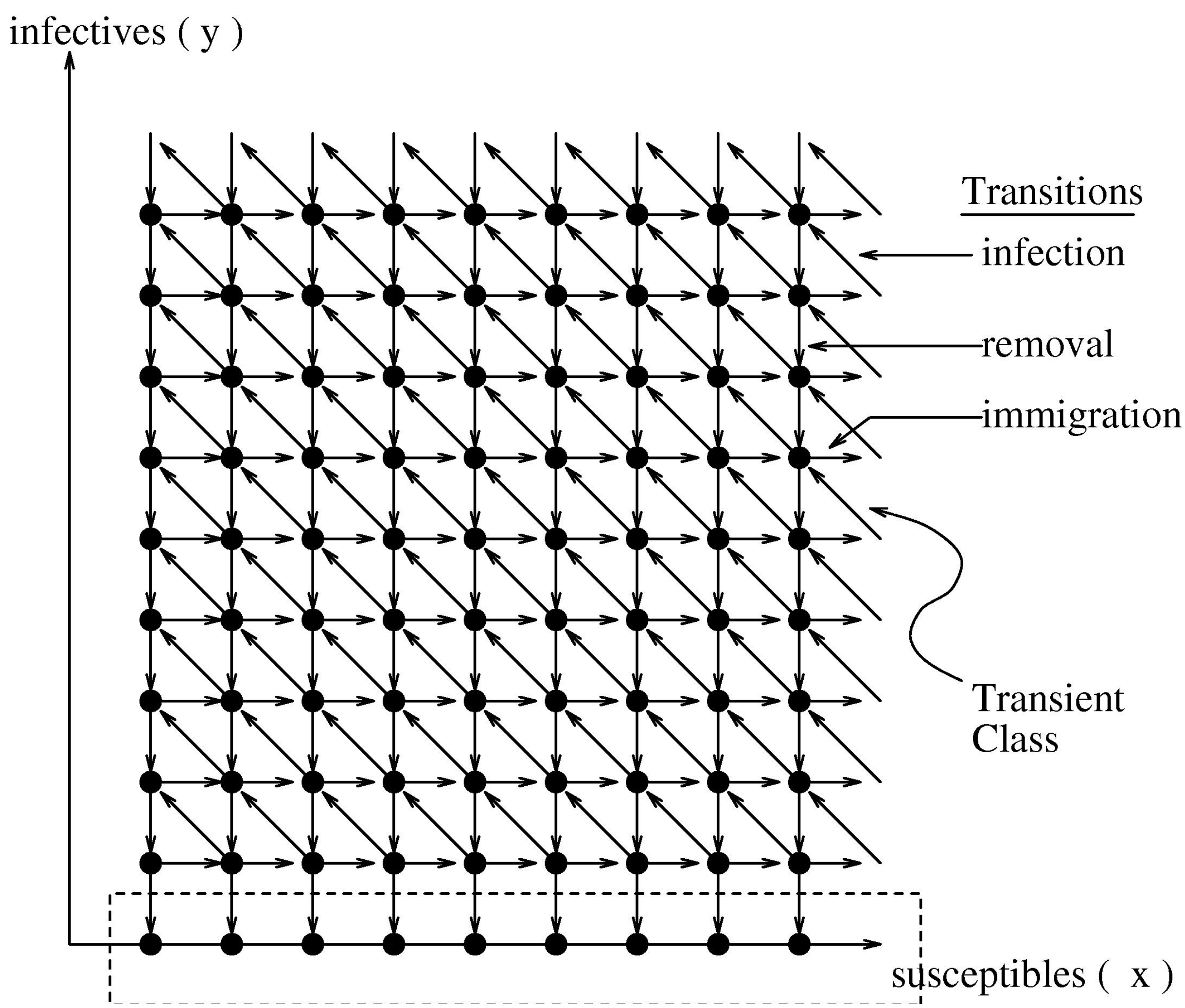
$$S = \{(x, y) : x, y = 0, 1, 2, \ldots\}$$

Transition rates $Q = (q_{ij}, i, j \in S)$:

if $i = (x, y)$, then

$$q_{ij} = \begin{cases} \beta xy & \text{if } j = (x-1, y+1), \\ \gamma y & \text{if } j = (x, y-1), \\ \alpha & \text{if } j = (x+1, y), \\ 0 & \text{otherwise.} \end{cases}$$

TRANSITION DIAGRAM



Transitions of the epidemic model

AN AUTO-CATALYTIC REACTION

Consider the following reaction scheme:

$$A \stackrel{X}{\to} B,$$

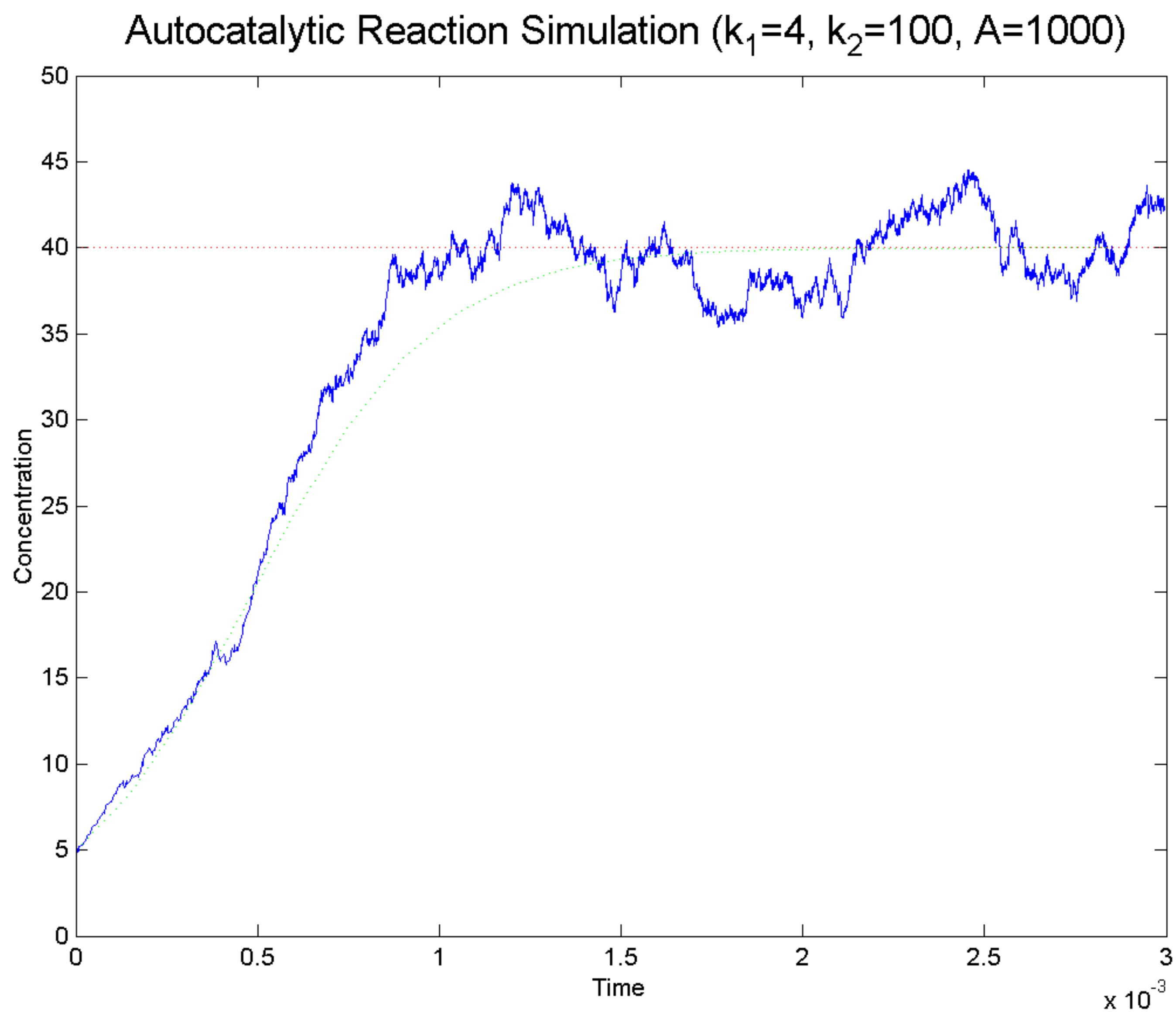
where X is a catalyst. Suppose that there are two stages, namely

$$A + X \stackrel{k_1}{\to} 2X \quad \text{and} \quad 2X \stackrel{k_2}{\to} B.$$

Let $X(t) =$ number of X molecules at time t.

Suppose that the concentration of A is held constant; let a be the number of molecules of A. The state space is $S = \{0, 1, 2, \dots\}$ and the transition rates are given by

$$q_{ij} = \begin{cases} k_1 a i & \text{if } j = i + 1, \\ k_2 \binom{i}{2} & \text{if } j = i - 2, \\ 0 & \text{otherwise.} \end{cases}$$



Autocatalytic Reaction Simulation (k1=4, k2=100, A=1000)
Concentration
Time
x 10-3
0
5
10
15
20
25
30
35
40
45
50
0
0.5
1
1.5
2
2.5
3

INGREDIENTS

The *state* at time t: $X(t) \in S = \{0, 1, 2, \dots\}$.

Transition rates $Q = (q_{ij}, i, j \in S)$: $q_{ij}\,(\geq 0)$, for $j \neq i$, is the transition rate from state i to state j and $q_{ii} = -q_i$, where $q_i = \sum_{j \neq i} q_{ij}\,(< \infty)$ is the transition rate out of state i.

Assumptions: Take 0 to be the sole absorbing state (that is, $q_{0j} = 0$). For simplicity, suppose that $C = \{1, 2, \dots\}$ is "irreducible" and that we reach 0 from C with probability 1.

State probabilities: $p(t) = (p_j(t), j \in S)$, where $p_j(t) = \Pr(X(t) = j)$.

Initial distribution: $a = (a_j, j \in S)$ $(a_0 = 0)$.

Forward equations: the state probabilities satisfy $p'(t) = p(t)Q$, $p(0) = a$. In particular, since $q_{0j} = 0$,

$$p_j'(t) = \sum_{i \in C} p_i(t) q_{ij}, \quad j \in S,\ t > 0.$$

THE STRUCTURE OF Q

Q has non-negative off-diagonal entries, non-positive diagonal entries, and zero row sums.

In the present setup we have, additionally, that (i) the first row is zero (because 0 is an absorbing state) and (ii) the first column has at least one positive entry (because we must be able to reach 0 from C).

Example. Birth-death processes

$$\begin{pmatrix} 0 & 0 & 0 & 0 & \dots \\ \mu_1 & -(\lambda_1+\mu_1) & \lambda_1 & 0 & \dots \\ 0 & \mu_2 & -(\lambda_2+\mu_2) & \lambda_2 & \dots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}$$

Example. The autocatalytic reaction

$$\begin{pmatrix} 0 & 0 & 0 & 0 & 0 & \dots \\ 0 & -k_1 a & k_1 a & 0 & 0 & \dots \\ k_2 & 0 & -(2k_1 a + k_2) & 2k_1 a & 0 & \dots \\ 0 & 3k_2 & 0 & -3(k_1 a + k_2) & 3k_1 a & \dots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}$$

MODELLING QUASI STATIONARITY

Recall that $S = \{0\} \cup C$, where 0 is an absorbing state and $C = \{1, 2, \dots\}$ is the set of transient states.

Conditional state probabilities: Define $m(t) = (m_j(t), j \in C)$ by

$$m_j(t) = \Pr(X(t) = j \,|\, X(t) \in C),$$

the chance of being in state j *given that the process has not reached* 0.

Question 1. Can we choose the initial distribution a in order that $m_j(t) = a_j$, $j \in C$, for all $t > 0$?

Question 2. Does $m(t) \to m$ as $t \to \infty$?

Definition. A distribution $m = (m_j, j \in C)$ satisfying $m(t) = m$ for all $t > 0$ is called a *quasi-stationary distribution*. If $m(t) \to m$ then m is called a *limiting-conditional distribution*.

SOME CALCULATIONS

For $j \in C$,

$$m_j(t) = \Pr(X(t) = j \mid X(t) \in C) = \frac{\Pr(X(t) = j)}{\Pr(X(t) \in C)} = \frac{p_j(t)}{\sum_{k \in C} p_k(t)} = \frac{p_j(t)}{1 - p_0(t)}$$

Therefore,

$$m_j'(t) = \frac{p_j'(t)}{1 - p_0(t)} + p_j(t)\frac{p_0'(t)}{(1 - p_0(t))^2} = \frac{p_j'(t)}{1 - p_0(t)} + m_j(t)\frac{p_0'(t)}{1 - p_0(t)} = \sum_{k \in C} m_k(t) q_{kj} + m_j(t) \sum_{k \in C} m_k(t) q_{k0}.$$

$$\boxed{m_j'(t) = \sum_{k \in C} m_k(t) q_{kj} + m_j(t) \sum_{k \in C} m_k(t) q_{k0}.}$$

Since $\sum_{j \in S} q_{ij} = 0$, this can be written $m'(t) = m(t)A - c_t m(t)$, where $c_t = m(t)A1$ and A is the restriction of Q to C.

QUASI-STATIONARY DISTRIBUTIONS

Since a is the initial distribution (with $a_0 = 0$),

$$p_j(t) = \sum_{i \in C} a_i p_{ij}(t), \quad j \in C,\ t < 0,$$

where $p_{ij}(t) = \Pr(X(t) = j | X(0) = i)$. Therefore, if m is a quasi-stationary distribution, then

$$\sum_{i \in C} m_i p_{ij}(t) = g(t) m_j, \quad j \in C,\ t > 0,$$

where $g(t) = \sum_{i \in C} p_i(t)$. It is easy to show that g satisfies: $g(s+t) = g(s)g(t)$, $s, t \geq 0$, and $0 < g(t) < 1$. Thus, $g(t) = e^{-\mu t}$, for some $\mu > 0$. The converse is also true.

Proposition. A probability distribution $m = (m_j, j \in C)$ is a quasi-stationary distribution if and only if, for some $\mu > 0$, m is a μ-invariant measure, that is

$$\sum_{i \in C} m_i p_{ij}(t) = e^{-\mu t} m_j, \quad j \in C,\ t \geq 0. \qquad (1)$$

CAN WE DETERMINE m from Q?

Rewrite (1) as

$$\sum_{i\in C:\, i\neq j} m_i p_{ij}(t) = \Big((1 - p_{jj}(t)) - (1 - e^{-\mu t})\Big) m_j$$

and use the fact that q_{ij} is the right-hand derivative of $p_{ij}(\cdot)$ near 0. On dividing by t and letting $t \downarrow 0$, we get (formally)

$$\sum_{i\in C:\, i\neq j} m_i q_{ij} = (q_j - \mu) m_j, \quad j \in C,$$

or, equivalently,

$$\sum_{i\in C} m_i q_{ij} = -\mu m_j, \quad j \in C. \qquad (2)$$

Accordingly, we shall say that m is a μ-invariant measure for Q whenever (2) holds.

Proposition. If m is a quasi-stationary distribution then, for some $\mu > 0$, m is a μ-invariant measure for Q.

IS THE CONVERSE TRUE?

Suppose that, for some $\mu > 0$, m is a μ-invariant measure for Q, that is

$$\sum_{i \in C} m_i q_{ij} = -\mu m_j, \quad j \in C.$$

Is m a quasi-stationary distribution?

Sum this equation over $j \in C$: we get (formally)

$$\sum_{i \in C} m_i q_{i0} = -\sum_{i \in C} m_i \sum_{j \in C} q_{ij} = -\sum_{j \in C} \sum_{i \in C} m_i q_{ij}$$

$$= \mu \sum_{j \in C} m_j = \mu.$$

Theorem. Let $m = (m_j, j \in C)$ be a probability distribution over C and suppose that m is a μ-invariant measure for Q. Then, $\mu \leq \sum_{j \in C} m_j q_{j0}$ with equality if and only if m is a quasi-stationary distribution.

AN EXAMPLE

The birth-death-catastrophe process. Let $S = \{0, 1, 2, \dots\}$ and suppose that

$$\begin{array}{rc}
q_{i,i+1} = a\rho i, & i \geq 0, \\
q_{i,i} = -\rho i, & i \geq 0, \\
q_{i,i-k} = \rho i b_k, & i \geq 2,\ k = 1, 2 \dots i-1, \\
q_{i,0} = \rho i \sum_{k=i}^{\infty} b_k, & i \geq 1,
\end{array}$$

where $\rho, a > 0$, $b_i > 0$ for at least one $i \geq 1$ and $a + \sum_{i=1}^{\infty} b_i = 1$. Jumps occur at a constant "per-capita" rate ρ and, at a jump time, a birth occurs with probability a, or otherwise a catastrophe occurs, the size of which is determined by the probabilities b_i, $i \geq 1$.

Clearly, 0 is an absorbing state and $C = \{1, 2, \dots\}$ is an irreducible class.

So, does the process admit a quasi-stationary distribution?

CALCULATIONS

On substituting the transition rates into the equations $\sum_{i \in C} m_i q_{ij} = -\mu m_j$, $j \in C$, we get:

$$-(\rho - \mu) m_1 + \sum_{k=2}^{\infty} k \rho b_{k-1} m_k = 0,$$

and, for $j \geq 2$,

$$(j-1)\rho a m_{j-1} - (j\rho - \mu) m_j + \sum_{k=j+1}^{\infty} k \rho b_{k-j} m_k = 0.$$

If we try a solution of the form $m_j = t^j$, the first equation tells us that $\mu = -\rho(f'(t) - 1)$, where

$$f(s) = a + \sum_{i \in C} b_i s^{i+1}, \qquad |s| \leq 1,$$

and, on substituting both of *these* quantities in the second equation, we find that $f(t) = t$. This latter equation has a unique solution σ on $[0, 1]$. Thus, by setting $t = \sigma$ we obtain a positive μ-invariant measure $m = (m_j, j \in C)$ for Q, which satisfies $\sum_{j \in C} m_j = 1$ whenever $\sigma < 1$.

The condition $\sigma < 1$ is satisfied only in the subcritical case, that is, when (the drift) $D = a - \sum_{i \in C} i b_i < 0$; this also guarantees that absorption occurs with probability 1.

Further, it is easy to show that $\sum_{i \in C} m_i q_{i0} = \mu$:

$$\begin{aligned} \sum_{i \in C} m_i q_{i0} &= \sum_{i=1}^{\infty} (1-\sigma)\sigma^{i-1} \rho i \sum_{k=i}^{\infty} b_k \\ &= \rho \sum_{k=1}^{\infty} b_k \sum_{i=1}^{k} (1-\sigma) i \sigma^{i-1} \\ &\vdots \\ &= \rho(1 - f'(\sigma)) = \mu. \end{aligned}$$

Proposition. The subcritical birth-death-catastrophe process has a geometric quasi-stationary distribution $m = (m_j,\ j \in C)$. This is given by

$$m_j = (1-\sigma)\sigma^{j-1}, \qquad j \in C,$$

where σ is the unique solution to $f(t) = t$ on the interval $[0, 1]$.

SOME RECENT TECHNOLOGY

Theorem. If the equations

$$\sum_{i \in C} y_i q_{ij} = \nu y_j, \quad j \in C,$$

have no non-trivial, non-negative solution such that $\sum_{i \in C} y_i < \infty$, for some (and then all) $\nu > 0$, then *all* μ-invariant probability measures for Q are quasistationary distributions.

[More generally, writing α_i for the probability of absorption starting in i, we have the following:

Theorem. If the equations

$$\sum_{i \in C} y_i q_{ij} = \nu y_j, \quad j \in C,$$

have no non-trivial, non-negative solution such that $\sum_{i \in C} y_i \alpha_i < \infty$, for some (and then all) $\nu > 0$, then *all* μ-invariant measures for Q satisfying $\sum_{i \in C} m_i \alpha_i < \infty$, are μ-invariant for P.]

COMPUTATIONAL METHODS

Finite S. Mandl (1960) showed that the restriction of Q to C has eigenvalues with negative real parts and the one with maximal real part (called $-\mu$ above) is real and has multiplicity 1, and, the corresponding left eigenvector $l = (l_j, j \in C)$ has positive entries; this is, of course, a μ-invariant measure for Q (unique up to constant multiples). Since S is finite, the quasi-stationary distribution $m = (m, i \in C)$ exists and is given by

$$m_j = \frac{l_j}{\sum_{k \in C} l_k}, \quad j \in C.$$

Infinite S. Truncate the restriction of Q to an $n \times n$ matrix, $Q^{(n)}$, and construct a sequence, $\{l^{(n)}\}$, of eigenvectors and hope that this converges to a μ-invariant measure l for Q, et cetera.

HOW SHOULD WE EVALUATE m?

Consider once again our epidemic model.

First truncate C to

$$C_N = \{(x, y) : x = 0, \ldots, N-1; y = 1, \ldots, N\}$$

and restrict Q to C_N. Use the transformation $i = x + N(y-1)$ to convert the restricted q-matrix into an $n \times n$ matrix, $Q = (q_{ij}, i, j = 0, 1, \ldots, n-1)$, where $n = N^2$.

Evaluation of the eigenvectors of Q is not completely trivial. For example, if (as well shall assume) $N = 100$, that is $n = 10^4$, Q needs 400 Mbytes of storage.

However, for N large, this matrix is large and sparse. Does this help?

THE ARNOLDI METHOD

We need to solve $Ax = \lambda x$, where $A = Q^T$.

Using an initial estimate of x, the basic Arnoldi method produces an $m \times m$ (upper-Hessenberg) matrix H_m and an $n \times m$ matrix V_m with

$$V_m^T A V_m = H_m,$$

and such that if z_m is an eigenvector of H_m, then, for m large, $V_m z_m$ is close to an eigenvector of A.

We solve for z_m using standard (dense-matrix) methods.

AN ITERATIVE ARNOLDI METHOD

Take m small (we found that $m = 20$ worked best). Then, using an initial estimate v_1 of the eigenvector x, apply the basic Arnoldi method (to obtain H_m and V_m) and set $\hat{\lambda}$ to be the dominant eigenvalue of H_m if this is real, or set $\hat{\lambda}$ equal to zero otherwise.

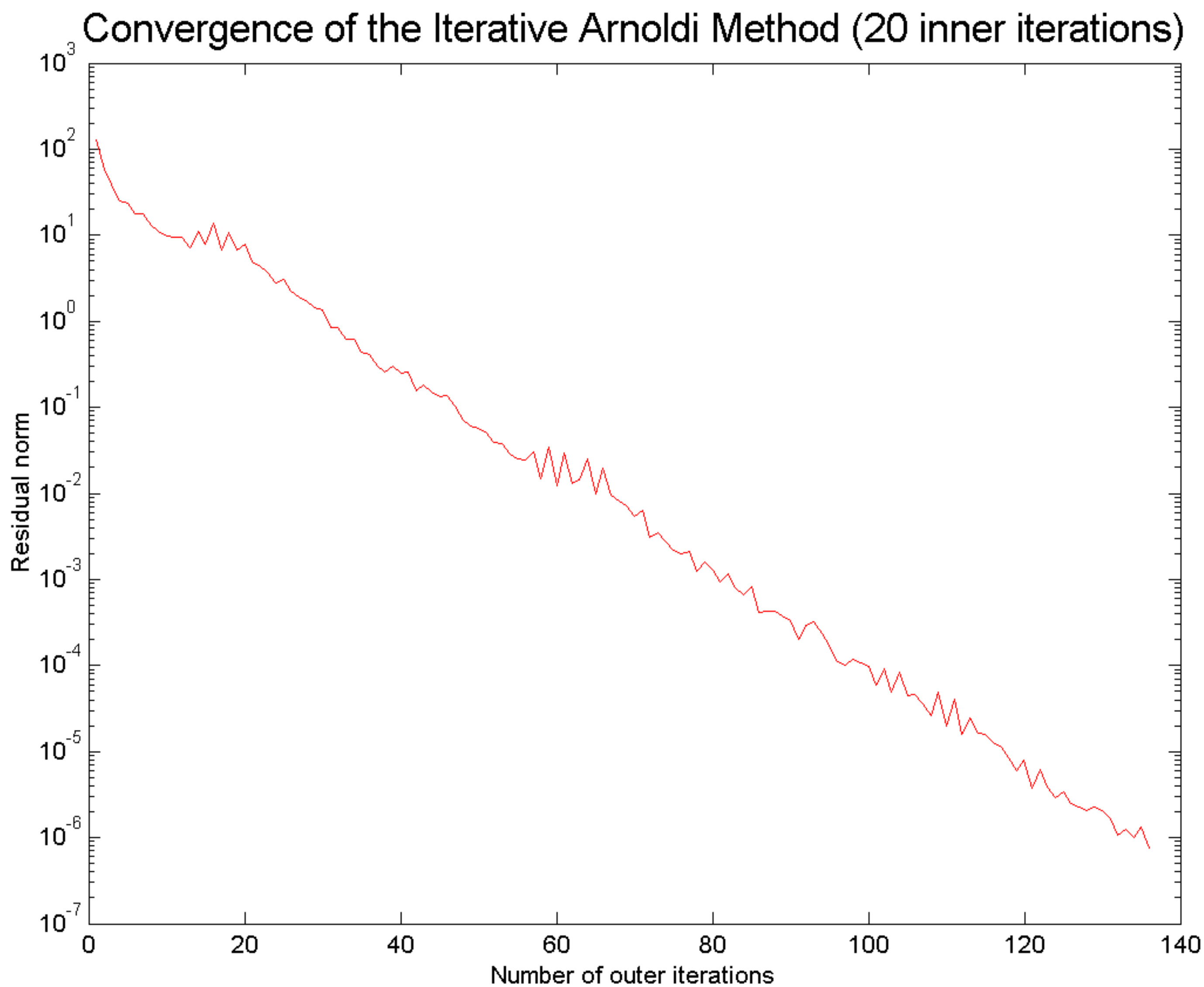
Now solve

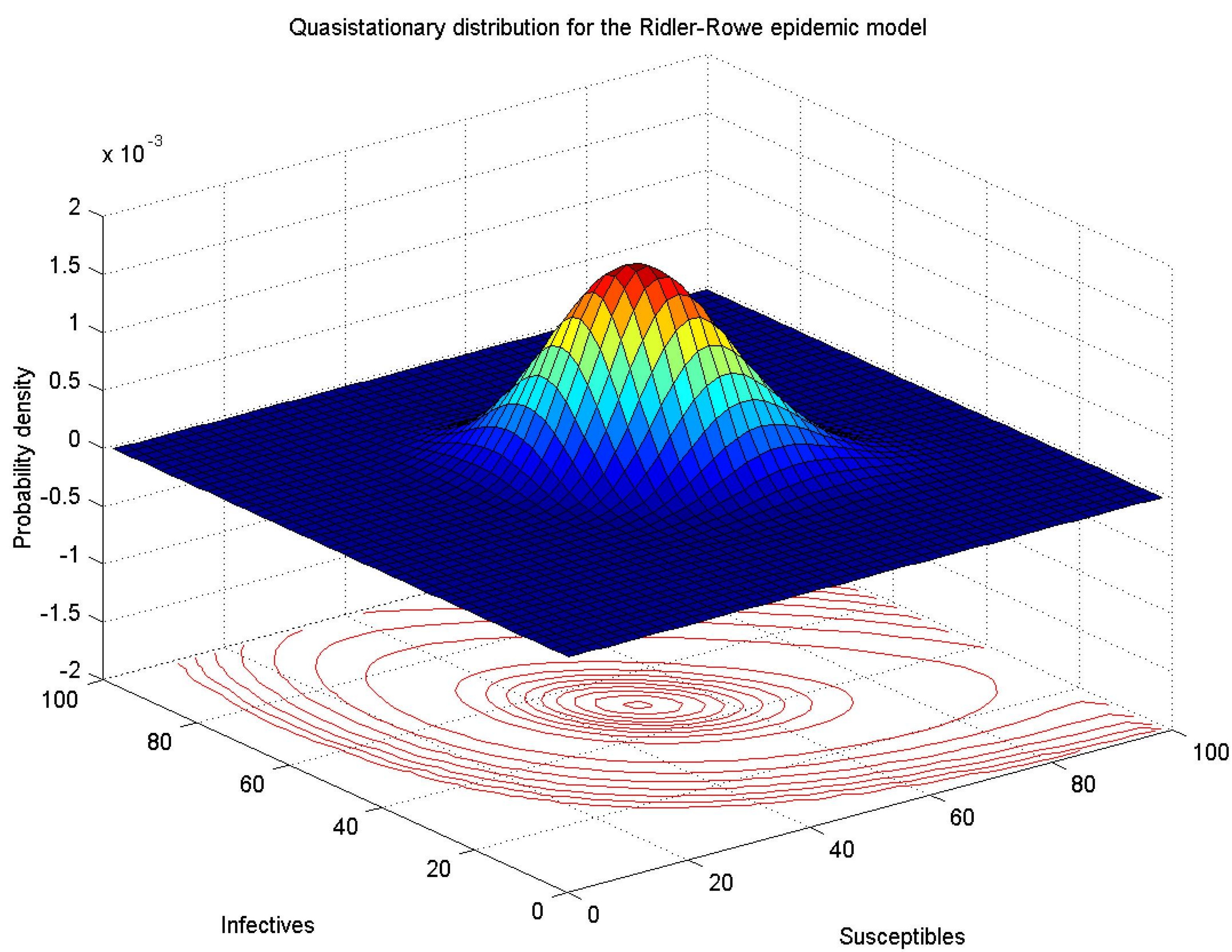
$$(H_m - \hat{\lambda} I) u_1 = z$$

with z chosen at random and repeat the procedure with a new initial estimate, given by

$$v_1 = V_m u_1 / \|V_m u_1\|_2.$$

Continue until the residual, $\|Av_1 - \hat{\lambda} v_1\|_2$, is sufficiently small.


Convergence of the Iterative Arnoldi Method (20 inner iterations)
Residual norm
Number of outer iterations
10^3
10^2
10^1
10^0
10^-1
10^-2
10^-3
10^-4
10^-5
10^-6
10^-7
0
20
40
60
80
100
120
140


Quasistationary distribution for the Ridler-Rowe epidemic model
x 10^-3
2
1.5
1
0.5
0
-0.5
-1
-1.5
-2
Probability density
100
80
60
40
20
0
Infectives
0
20
40
60
80
100
Susceptibles