Centrum voor Wiskunde en Informatica
Centre for Mathematics and Computer Science

H. Roozen

Numerical construction of rays and confidence contours in stochastic population dynamics

Department of Applied Mathematics Note AM-N8602 August

The Centre for Mathematics and Computer Science is a research institute of the Stichting Mathematisch Centrum, which was founded on February 11, 1946, as a nonprofit institution aiming at the promotion of mathematics, computer science, and their applications. It is sponsored by the Dutch Government through the Netherlands Organization for the Advancement of Pure Research (Z.W.O.).

Numerical Construction of Rays and Confidence Contours in Stochastic Population Dynamics

H. Roozen
Centre for Mathematics and Computer Science
P.O. Box 4079, 1009 AB Amsterdam, The Netherlands

Consider a stochastic system with small stochastic perturbations in which the associated deterministic system has a stable equilibrium. The (quasi-) stationary forward Fokker-Planck equation is solved by the WKB-method, leading to a system of ray equations. This technical note deals with the numerical solution of the ray equations. The methods which are described here have been applied to stochastic birth-death models [1]. This technical note is a supplement to the paper [1].

1980 Mathematics Subject Classification : 60J70, 60J60.
Key Words and Phrases : Ray method, confidence contours.

1. Introduction

We consider the n-dimensional stochastic system which is described by the (quasi-) stationary Fokker-Planck (or forward Kolmogorov) equation:

$$0 = -\sum_{i=1}^{n} \frac{\partial}{\partial x_i}[b_i(x)P_s(x)] + \frac{\epsilon}{2}\sum_{i=1}^{n}\sum_{j=1}^{n} \frac{\partial^2}{\partial x_i \partial x_j}[a_{ij}(x)P_s(x)] \,, \tag{1.1}$$

in which b is the deterministic vector field, a the symmetric positive (semi-) definite diffusion matrix, and ϵ a small parameter. It is assumed that in a bounded region R of the state space x, the deterministic system

$$\frac{dx}{dt} = b(x) \tag{1.2}$$

has a single stable equilibrium. Without loss of generality this equilibrium is positioned at the origin. With respect to the behaviour of the deterministic vector field at the boundary S of the region R, different cases can be distinguished:

a) $b\,.\,\nu \leq 0$, in which ν is the outward normal at S. The asymptotic theory for small ϵ is set out in the paper [2].
b) $b\,.\,\nu = 0$ without critical points on S. The asymptotic theory can be found in [3].
c) $b\,.\,\nu = 0$ with critical points on S. For the asymptotic theory, see [4].

The asymptotic theories for small ϵ yield expressions for the most probable exit point $x^* \in S$ from the region R, and the expected time of exit from the region R. In the asymptotic theories the diffusion is not allowed to vanish at the boundary S. The asymptotic analysis for a simple one-dimensional system in which both the deterministic vector field and the diffusion vanish at the boundary is given in [5].

To the solution of (1.1) a simple WKB-Ansatz [6] is made:

$$P_s(x) = Ce^{\frac{-Q(x)}{\epsilon}} \,. \tag{1.3}$$

Substitution in (1.1) leads in largest order of ϵ to the eikonal equation:

Note AM-N8602
Centre for Mathematics and Computer Science
P.O. Box 4079, 1009 AB Amsterdam, The Netherlands

$$0 = \sum_i b_i(x)\frac{\partial Q}{\partial x_i} + \sum_{i,j}\frac{1}{2}a_{ij}(x)\frac{\partial Q}{\partial x_i}\frac{\partial Q}{\partial x_j} . \tag{1.4}$$

This is a Hamilton-Jacobi equation and can be written as $H(x,p) = 0$, in which H is the Hamiltonian

$$H(x,p) = \sum_i b_i p_i + \sum_{i,j}\frac{1}{2}a_{ij}p_i p_j , \tag{1.5}$$

with $p_i = \partial Q/\partial x_i$. The corresponding system of ordinary differential equations is:

$$\frac{dx_i}{ds} = \frac{\partial H}{\partial p_i} = b_i + \sum_j a_{ij}p_j , \quad (i=1,2,..., n) \tag{1.6a}$$

$$\frac{dp_i}{ds} = -\frac{\partial H}{\partial x_i} = -\sum_j \frac{\partial b_j}{\partial x_i}p_j - \sum_{j,k}\frac{1}{2}\frac{\partial a_{jk}}{\partial x_i}p_j p_k , \quad (i=1,2,..., n) \tag{1.6b}$$

$$\frac{dQ}{ds} = -H(x,p) + \sum_i \frac{dx_i}{ds}p_i = \sum_{i,j}\frac{1}{2}a_{ij}p_i p_j , \tag{1.6c}$$

in which s is a parameter along the characteristics. The projection of a characteristic on the x-space is called a ray. The system (1.6) is called the system of ray equations. It can be considered as a dynamical system in which Q and the elements of x and p are the state variables. Q is passive in the sense that it depends on the other state variables, while the other state variables do not depend on Q. If desired, Q could be omitted from the system and be computed afterwards from the values of x and p along the characteristic. The dynamical system (1.6) is assumed to have the stable equilibrium

$$\begin{aligned} &x = p = 0 , \\ &Q = 0 . \end{aligned} \tag{1.7}$$

The projection of this equilibrium point on the x-space coincides with the stable equilibrium point of the deterministic system. The value of Q is zero at the equilibrium point. All characteristics start in a close neighbourhood of the equilibrium point. As is seen from equation (1.6c), the value of Q along a characteristic is nondecreasing. The use of the function Q is in the following:

i) In the construction of confidence contours. The confidence contour of probability z $(0 \leq z \leq 1)$ encloses the smallest region in the x-space where with probability z the system can be found. By the assumption (1.3) the confidence contours are $(n-1)$-dimensional surfaces in the x-space on which Q has a constant value. It must be noted that for type c boundaries and for absorbing boundaries the WKB-Ansatz is not valid near the boundary.
ii) For type a boundaries to find the most probable exit point and the expected exit time from the region R. The asymptotic theory in [2] shows that the point x^* at S which has the lowest Q-value is the most probable point of exit and that the expected exit time is expressed in the value of Q at x^* by $T \sim e^{\frac{Q(x^*)}{\epsilon}}$.

Various ways of solving the system of ray equations numerically are discussed below.

2. The initial value approach

The initial point $x(s=0)$ of a ray is chosen close to the equilibrium (1.7). A local analysis in the neighbourhood of the equilibrium yields the values for $p(s=0)$ and $Q(s=0)$. In this local analysis, Q is approximated by a quadratic form

$$Q(x) \approx \frac{1}{2}x^t P x , \tag{2.1}$$

in which t denotes the transpose and P is a symmetric matrix. It follows that

$$p = \frac{dQ}{dx} \approx Px . \tag{2.2}$$

The deterministic vector field b is approximated by its linearization at $x=0$:

$$b \approx Bx \,, \tag{2.3}$$

in which $B=(\partial b_i(0)/\partial x_j)$. Substitution of (2.2) and (2.3) in the eikonal equation gives:

$$PAP + PB + B^t P = 0 \,, \tag{2.4}$$

in which the matrix A is given by $A = (a_{ij}(0))$. Left and right multiplication of (2.4) with $S=P^{-1}$ gives:

$$A + BS + SB^t = 0 \,. \tag{2.5}$$

If the matrices S and A are written colomnwise as vectors, a linear system with n^2 equations is obtained, which can be solved for S. The matrix P is obtained by inversion of S. All eigenvalues of B are negative because of the stability of the equilibrium of the deterministic system. Consequently, the last two operations can be carried out. The elements of the matrix P can be substituted in expressions (2.2) and (2.3), resulting in the approximations for $p(s=0)$ and $Q(s=0)$.

The ray equations are solved numerically by a routine for solving a system of ordinary differential equations in first order form, with initial conditions. Such routines can be found for example in the NAG-library [7]. The solution $x(s)$, $p(s)$, $Q(s)$ is obtained along the characteristic defined by the initial point $x(s=0)$. In cases that one is interested in the ray starting from a particular point where the values of p , x and Q are known (or can be approximated), the initial value method performs well and by using an appropriate numerical routine, the solution can be obtained with a high accuracy. There is no control however, over the way the ray develops through the x-space. Generally, there is a strong dependence on the choice of the initial point. Thus, the method is not well suited for the construction of confidence contours. This has been demonstrated for a two-dimensional stochastic model in [1, p. 17-18]. In some numerical integration routines there is the possibility of using a termination criterion based on the value of one of the state variables. If it is desired to terminate the computation at a specific value of Q, then the treatment of Q as a state variable is advantageous.

3. The boundary value method

In this approach $n+1$ conditions are imposed at the beginning of the ray and n conditions at the end of the ray:

$$\begin{aligned} &s \to -\infty: \quad Q=0,\ x=0\,, \\ &s=0: \qquad x=e\,, \end{aligned} \tag{3.1}$$

where e is the endpoint which can be chosen freely. In the numerical computations the limit $s \to -\infty$ is replaced by $s=-s^*$, with s^* a sufficiently large number. The problem is solved by using the NAG-routine D02RAF, ment for a system of ordinary first order differential equations with boundary conditions. The routine uses a deferred correction technique and Newton iteration. On a grid of s-values, an initial estimate to the solution has to be given, from which the routine iteratively tries to find the solution. The initial estimate for the x-coördinates on the grid follows from a linear interpolation between the coördinates of the equilibrium and the endpoint. The initial estimate for the corresponding values of p and Q is based on the local analysis formulas (see section 2). An alternative way to obtain initial estimates is to use the known values along a characteristic close tot the desired characteristic.

For $s \to -\infty$ the condition $x=0$ has been imposed and not the condition $p=0$. The motivation for doing this is explained by means of an example.

Example 1. The one-dimensional stochastic system defined by

$$b(x) = x(1-x), \quad a(x) = 2x \tag{3.2}$$

is considered. The deterministic system has an unstable equilibrium at $x=0$ and a stable equilibrium

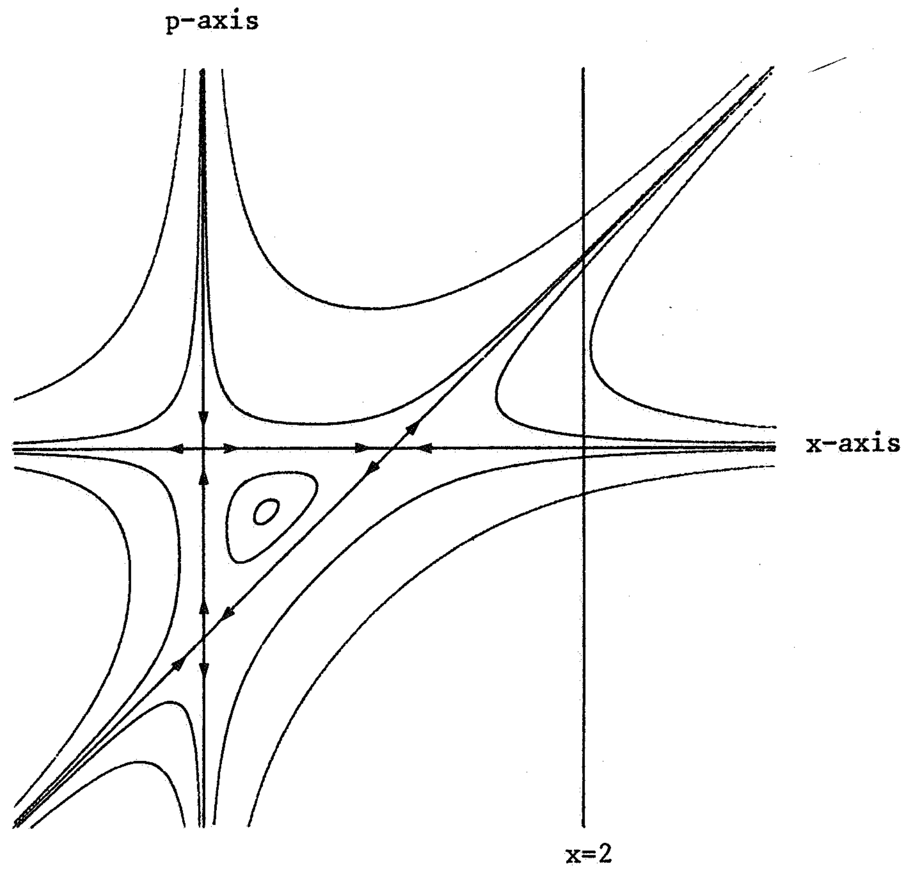

FIGURE 1. Some trajectories of the system (3.3) in the x,p-state space.

at $x=1$. A solution is sought in the form of the WKB-Ansatz, Q having a minimum at $x=1$. The system of ray equations yields:

$$\frac{dx}{ds} = x(1-x) + 2xp\ , \tag{3.3a}$$

$$\frac{dp}{ds} = (2x-1)p - p^2\ , \tag{3.3b}$$

$$\frac{dQ}{ds} = xp^2\ . \tag{3.3c}$$

The system (3.3ab) has the following equilibrium points:

$$\begin{aligned} &x=1,\ \ p=0\ ,\\ &x=0,\ \ p=0\ ,\\ &x=0,\ \ p=-1\ ,\\ &x=\tfrac{1}{3},\ p=-\tfrac{1}{3}\ . \end{aligned} \tag{3.4}$$

Trajectories of the system (3.3ab) are depicted in fig.1. The local analysis in the neighbourhood of $x=1, p=0$ shows that the solution of this example is situated along the line $p=x-1$. Linearization of this system at $x=1, p=0$ gives:

$$\begin{pmatrix} \frac{dx}{ds} \\ \frac{dp}{ds} \end{pmatrix} \approx \begin{pmatrix} -1 & 2 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} x-1 \\ p \end{pmatrix} . \tag{3.5}$$

The matrix has the following eigenvalues and corresponding eigenvectors:

$$\lambda_1 = -1, \quad w_1 = \begin{pmatrix} 1 \\ 0 \end{pmatrix} , \tag{3.6a}$$

$$\lambda_2 = 1, \quad w_2 = \begin{pmatrix} 1 \\ 1 \end{pmatrix} . \tag{3.6b}$$

So in the neighbourhood of the equilibrium $x=1, p=0$ there is a stable manifold corresponding to the first eigenvalue and eigenvector and an unstable manifold corresponding to the second eigenvalue and eigenvector. In this example the end of the ray is for example specified by the condition:

$$s = 0 : \quad x = 2\ . \tag{3.7}$$

From fig. 1 it is apparent that by the condition

$$s \to -\infty : \quad p = 0 \tag{3.8}$$

the solution is not uniquely determined. Apart from the desired solution along the characteristic $p=x-1$, there is an infinite number of other solutions satisfying condition (3.7) as well as condition (3.8). In contrast, the condition

$$s \to -\infty : \quad x = 1 \tag{3.9}$$

together with condition (3.7) determine the solution uniquely. From this example we see that the condition for $s=-\infty$ must not be such that it determines a surface in the x, p-space which coincides with the stable manifold at the equilibrium point.

REMARK

Apart from this, fig. 1 exhibits an interesting feature. The region enclosed by the trajectories connecting the equilibrium points $(x=1, p=0)$, $(x=0, p=-1)$ and $(x=0, p=0)$ contains periodic orbits.

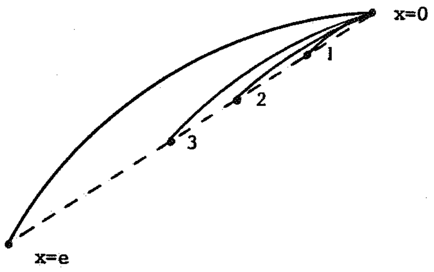

FIGURE 2. Construction of a ray (growing ray method).

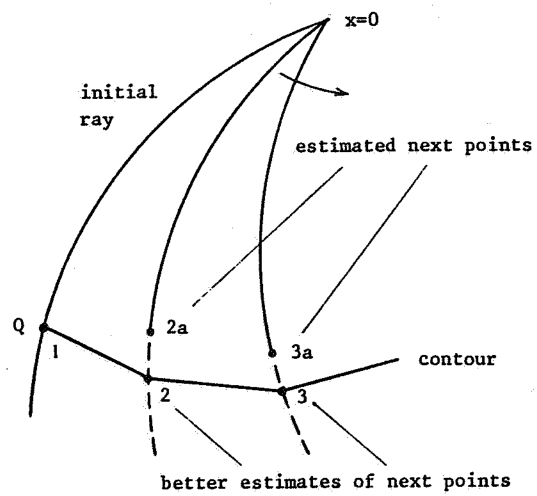

FIGURE 3. Construction of a confidence contour.

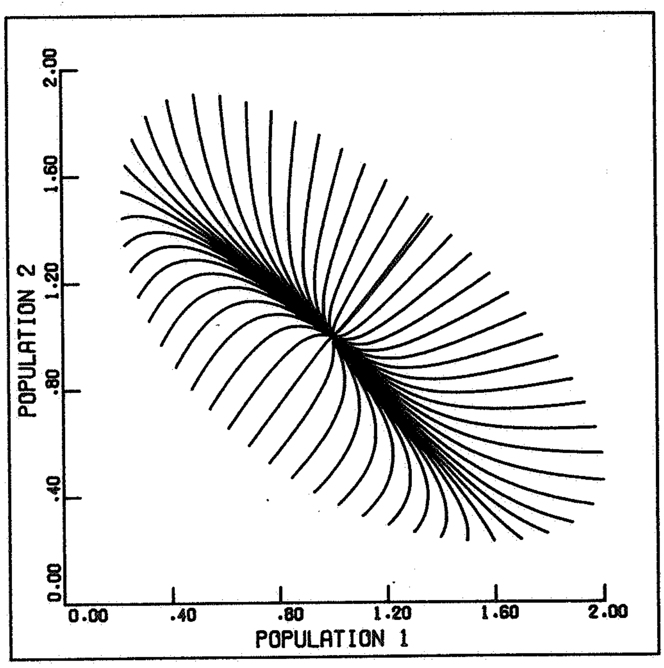

FIGURE 4. The rays used in the construction of a confidence contour. The confidence contour is obtained by connecting the end points of the rays.

Along such an orbit s increases and by (3.3c) also Q increases. After every rotation, the value of Q takes a positive jump. In this region Q is a multivalued function of x. In the region $0<p<x-1$ $Q(x)$ is two-valued.

The solution we are interested in is situated along $p=x-1$ (which is a straight line; generally in one dimensional stochastic systems we have to do with a *curve*). Small errors occur in the initial values of the ray variables and during the integration of the ray equations by the initial value method. As a consequence the line $p=x-1$ is not followed exactly. In the limit $s\to\infty$, instead of approaching the point $x=0$, $p=-1$ asymptotically, a trajectory close to $p=x-1$ is followed, which in the neighbourhood of this point curves upward or downward along the p-axis. When this happens the computation can be terminated because the results have lost significance. We see that 1) the initial value method is not well suited for the construction of a characteristic connection two equilibrium points and 2) the picture of the state space is helpfull in understanding the behaviour of the numerical solution of the ray equations.

Let's go back to the original system of ray equations (1.6). Linearization of the equations (1.6ab) at the equilibrium $x=0$, $p=0$ yields:

$$\begin{bmatrix} \frac{dx}{ds} \\ \frac{dp}{ds} \end{bmatrix} = \begin{bmatrix} B & A \\ 0 & -B^t \end{bmatrix} \begin{bmatrix} x \\ p \end{bmatrix}, \tag{3.10}$$

in which the matrices A and B are given by the values of (a_{ij}) and $(\partial b_i/\partial x_j)$ at the equilibrium $x=0$, $p=0$. Let the eigenvalues of the linearized deterministic system at $x=0$ be given by λ_i $(i=1,2,..., n)$ and the corresponding eigenvectors by w_i. By the assumption of stability of the deterministic equilibruim, the real parts of the eigenvalues are negative. The eigenvalues of the matrix in (3.10) are given by $\pm\lambda_i$ $(i=1,2,..., n)$. There is a stable manifold at $x=0, p=0$ of dimension n formed by the eigenvectors corresponding to the eigenvalues with negative real part, and an unstable manifold of dimension n formed by the eigenvectors corresponding to the eigenvalues with positive real part. The eigenvectors corresponding to the eigenvalues with negative real part are given by $(w_i^t, 0^t)^t$. When the conditions for $s\to-\infty$ are chosen as:

$$s\to-\infty : x = 0 \qquad \text{(and of course ,} Q = 0) \tag{3.11}$$

then the surface $(0^t, p^t)^t$ in the x, p-space is introduced which is perpendicular to the stable manifold at $x=0$, $p=0$. Thus, by this choice of the conditions, the kind of non-uniqueness as discussed in the example 1 does not occur.

Construction of a single ray.

The following discussion is based on the experience with the two-dimensional population models described in [1]. Other applications may require slight adaptations. The ray to be constructed is determined by the boundary conditions (3.1). The NAG-routine D02RAF has been used without the continuation facility. The grid consisted of 64 equidistant (in the parameter s) points. Experience has shown that the performance of the boundary value method depends critically on a sufficient number of grid points. The magnitude of s^* is less critical. The parameter tol, which expresses the maximum absolute deviation of the computed value from the true value in each component of the solution, was set equal to .01. The Jacobians which have to be computed were based on the exact analytical expressions. However, at an early stage of programming, it may be convenient to use the facility by which the Jacobians are approximated numerically. The initial estimate for the x-coordinates on the grid was based on a linear interpolation between the coordinates of the equilibrium point and the endpoint. The initial Q- and p-values were derived by the local analysis.

Only when the endpoint is close to the equilibrium point the solution is obtained. If not, the initial estimate is not sufficiently accurate and the routine fails. Rays with endpoints far from the equilibrium point are constructed successfully by one of the following methods.

i) *Growing ray method.*
A line is drawn from the equilibrium point to the endpoint. At point 1 on this line close to the equilibrium, the solution is obtained by applying the routine. The solution for the ray to point 1 is used as an initial estimate for the ray to point 2 on the line. The solution for the ray to point 2 is used as initial estimate for the ray to point 3, etc. The procedure is repeated until the point $x=e$ has been reached. See fig.2.

ii) *Neighbouring ray method.*
An alternative method is to construct a ray passing close to $x=e$ by the initial value method and using the values along this ray as initial estimate to the desired ray through $x=e$.

Construction of a confidence contour.
This is treated most easily for $n=2$. The generalization to arbitrary n is straightforward. A single ray is constructed, for example by the initial value method. The precise course of the ray is immaterial, but the ray must contain the Q-value corresponding to the desired contour. The point on the ray at which this value is attained is the first point of the contour. Moreover, the values of $p_1=\partial Q/\partial x_1$ and $p_2=\partial Q/\partial x_2$ are known at this point. An arbitrary but small distance d is specified. Based on the values of p_1 and p_2 an estimate of a second point $2a$ of the contour can be made, lying a distance d away from the first point of the contour. The ray with endpoint $2a$ is then computed. The known values along the first ray are used as initial estimate to the solution corresponding to the second ray. From the solution of the second ray a better estimate can be made of the position of the second point of the contour, which will be close to the point $2a$. By connecting this point with the first point we have obtained a small segment of the contour. The procedure is repeated for obtaining the following rays. See fig. 3. A mechanism must be built in to assure that a clockwise (or anti-clockwise) direction is followed. The procedure terminates after a complete rotation. A result of this procedure for a 2-dimensional stochastic population model as treated in [1] is shown in fig. 4.

Construction of the ray connecting equilibria.
The ray connecting the stable equilibrium point of the deterministic system with another equilibrium point of the deterministic system is constructed as follows. First consider the one-dimensional stochastic system of example 1. This system has the equilibrium point $x=0$, $p=-1$, which is connnected by the characteristic $p=x-1$ to the equilibrium $x=1$, $p=0$. It is easily seen from fig. 1 that this characteristic can be constructed by starting in a close neighbourhood of $x=1$, $p=0$ at the unstable manifold and solving the system of ray equations (3.3) by the initial value method. The equilibrium $x=0$, $p=-1$ is then approached along its stable manifold.

Next consider the two dimensional system:

EXAMPLE 2

$$\begin{aligned} b_1(x) &= x_1(3-2x_1-x_2)\,, \\ b_2(x) &= x_2(1+x_1-2x_2)\,, \\ a_1(x) &= x_1(1+x_1+x_2)\,, \\ a_2(x) &= x_2(1+x_1+x_2)\,, \end{aligned} \tag{3.12}$$

which has the equilibrium points

$$\begin{aligned} &x_1 = 1, \quad x_2 = 1\,, \\ &x_1 = \tfrac{3}{2}, \quad x_2 = 0\,, \\ &x_1 = 0, \quad x_2 = \tfrac{1}{2}\,, \\ &x_1 = 0, \quad x_2 = 0\,. \end{aligned} \tag{3.13}$$

The equilibrium $x_1 = 1$, $x_2 = 1$ is stable. A WKB-Ansatz leads to the system of ray equations:

$$\frac{dx_1}{ds} = x_1(3-2x_1-x_2)+x_1(1+x_1+x_2)p_1 ,$$
$$\frac{dx_2}{ds} = x_2(1+x_1-2x_2)+x_2(1+x_1+x_2)p_2 , \tag{3.14a}$$

$$\frac{dp_1}{ds} = -(3-4x_1-x_2)p_1-x_2p_2-\frac{1}{2}(1+2x_1+x_2)p_1^2-\frac{1}{2}x_2p_2^2 ,$$
$$\frac{dp_2}{ds} = x_1p_1-(1+x_1-4x_2)p_2-\frac{1}{2}x_1p_1^2-\frac{1}{2}(1+x_1+2x_2)p_2^2 , \tag{3.14b}$$

$$\frac{dQ}{ds} = \frac{1}{2}x_1(1+x_1+x_2)p_1^2+\frac{1}{2}x_2(1+x_1+x_2)p_2^2 . \tag{3.14c}$$

Suppose we are interested in the ray connecting the point $x_1=1$, $x_2=1$ with $x_1=3/2$, $x_2=0$. Substitution of the coordinates of the latter point in equations (3.14ab) gives:

$$\frac{dx_1}{ds}=\frac{15}{4}p_1 ,$$
$$\frac{dx_2}{ds}=0 ,$$
$$\frac{dp_1}{ds}=3p_1-2p_1^2 , \tag{3.15}$$
$$\frac{dp_2}{ds}=\frac{3}{2}p_1-\frac{3}{4}p_1^2-\frac{5}{2}p_2-\frac{5}{4}p_2^2 .$$

The corresponding nontrivial equilibrium for the ray equations is given by

$$x_1=\frac{3}{2} ,$$
$$x_2=0 ,$$
$$p_1=0 , \tag{3.16}$$
$$p_2=-2 .$$

Linearization of the ray equations in the neighbourhood of this point gives

$$\begin{bmatrix} \frac{dx_1}{ds} \\ \frac{dx_2}{ds} \\ \frac{dp_1}{ds} \\ \frac{dp_2}{ds} \end{bmatrix} = \begin{bmatrix} -3 & -\frac{3}{2} & \frac{15}{4} & 0 \\ 0 & -\frac{5}{2} & 0 & 0 \\ 0 & 0 & 3 & 0 \\ 0 & -12 & \frac{3}{2} & \frac{5}{2} \end{bmatrix} \begin{bmatrix} x_1-\frac{3}{2} \\ x_2 \\ p_1 \\ p_2+2 \end{bmatrix} . \tag{3.17}$$

The eigenvalues of the matrix are:

$$\lambda_1 = -3 ,$$
$$\lambda_2 = -\frac{5}{2} ,$$
$$\lambda_3 = 3 , \tag{3.18}$$
$$\lambda_4 = \frac{5}{2} .$$

The eigenvectors corresponding to the negative eigenvalues are:

$$v_1 = \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix}, \quad v_2 = \begin{bmatrix} -3 \\ 1 \\ 0 \\ \frac{12}{5} \end{bmatrix}. \tag{3.19}$$

They span the stable manifold at $x_1=3/2$, $x_2=0$, $p_1=0$, $p_2=-2$. The equilibrium point $x_1=3/2$, $x_2=0$, $p_1=0$, $p_2=-2$, can be reached by trajectories only along this stable manifold. The endpoint of the ray is chosen close to $x_1=3/2$, $x_2=0$ on the stable manifold:

$$\begin{bmatrix} x_1^e \\ x_2^e \\ p_1^e \\ p_2^e \end{bmatrix} = \begin{bmatrix} \frac{3}{2} \\ 0 \\ 0 \\ -2 \end{bmatrix} + \alpha v_1 + \beta v_2 , \tag{3.20}$$

in which the superscript e refers to the endpoint and α and β are small. The parameters α and β can be eliminated from the equations (3.20), resulting in the two endpoint conditions:

$$\begin{aligned} s \rightarrow +\infty : \ & p_1=0 , \\ & p_2=-2+\tfrac{12}{5}x_2 . \end{aligned} \tag{3.21}$$

The conditions at the beginning of the ray are derived analogously. At the beginning of the ray the ray equations possess the equilibrium:

$$\begin{aligned} x_1&=1 , \\ x_2&=1 , \\ p_1&=0 , \\ p_2&=0 . \end{aligned} \tag{3.22}$$

Linearization of the ray equations near this point gives:

$$\begin{bmatrix} \frac{dx_1}{ds} \\ \frac{dx_2}{ds} \\ \frac{dp_1}{ds} \\ \frac{dp_2}{ds} \end{bmatrix} = \begin{bmatrix} -2 & -1 & 3 & 0 \\ 1 & -2 & 0 & 3 \\ 0 & 0 & 2 & -1 \\ 0 & 0 & 1 & 2 \end{bmatrix} \begin{bmatrix} x_1-1 \\ x_2-1 \\ p_1 \\ p_2 \end{bmatrix}. \tag{3.23}$$

The eigenvalues of the matrix are:

$$\begin{aligned} \lambda_1 &= 2-i , \\ \lambda_2 &= 2+i , \\ \lambda_3 &= -2+i , \\ \lambda_4 &= -2-i . \end{aligned} \tag{3.24}$$

The eigenvectors corresponding to the eigenvalues with positive real part (λ_1 and λ_2) are:

$$v_1 = \begin{pmatrix} \frac{3}{4} \\ \frac{3}{4}i \\ 1 \\ i \end{pmatrix}, \; v_2 = \begin{pmatrix} \frac{3}{4} \\ -\frac{3}{4}i \\ 1 \\ -i \end{pmatrix}. \tag{3.25}$$

The ray must leave the equilibrium point $(1,1,0,0)'$ through the unstable manifold. The starting point is chosen close to the equilibrium on the unstable manifold:

$$\begin{pmatrix} x_1^b \\ x_2^b \\ p_1^b \\ p_2^b \end{pmatrix} = \begin{pmatrix} 1 \\ 1 \\ 0 \\ 0 \end{pmatrix} + c_1 \begin{pmatrix} \frac{3}{4} \\ \frac{3}{4}i \\ 1 \\ i \end{pmatrix} + c_2 \begin{pmatrix} \frac{3}{4} \\ -\frac{3}{4}i \\ 1 \\ -i \end{pmatrix}, \tag{3.26}$$

in which the superscript b refers to the begin point and c_1 and c_2 are small complex numbers. Eliminating c_1 and c_2 from (3.26) leads to the begin point conditions:

$$\begin{aligned} s \to -\infty : \; x_1 &= 1+\tfrac{3}{4}p_1 , \\ x_2 &= 1+\tfrac{3}{4}p_2 , \\ &\text{(and of course, } Q = 0) . \end{aligned} \tag{3.27}$$

The characteristic connecting the equilibrium points is determined by the conditions (3.21, 3.27). The problem is solved by the NAG-routine D02RAF. A good initial estimate to the solution is necessary in order for the routine to find the solution and can be obtained by constructing a growing ray or a neighbouring ray.

An alternative less elegant way to specify the boundary conditions is:

$$s \to -\infty: \quad x_1 = x_2 = 1, \quad Q = 0, \tag{3.27a}$$

$$s \to +\infty: \quad x_1 = 3/2, \quad x_2 = 0. \tag{3.21a}$$

This formulation has the advantage that no eigenvalues/vectors need to be calculated. Both formulations (3.21, 3.27) and (3.21a, 3.27a) lead to the same numerical results.

REMARK.
In the literature a classification of boundaries exists only for 1-dimensional stochastic systems, originating from Feller [8]. The one-dimensional analog of the two-dimensional system treated above has a boundary which is classified as an exit boundary. It can be reached from the interior of the state space within a finite time while the interior of the state space cannot be reached within a finite time from the boundary. A nontrivial stationary state does not exist. The equation (1.1) describes the quasi-stationary state, which often gives a good description of the stochastic process during some time. The WKB-Ansatz is not valid near the boundary. The two-dimensional system described above is related to a stochastic birth-death model with a discrete state space [1], which also has the property that the boundary can be reached but not be left again in a finite time. It is expected that for the problem above the WKB-Ansatz is not valid near the boundary and that statements based on the results can have only approximate validity.

Exit for problems with type a *boundaries.*
The determination of the most probable exit point x^* and the value of Q at this point can be carried out in several ways. In a variant of the boundary value method for confidence contours, rays are

constructed to points a small distance away from each other on the boundary at which exit is studied. The solution along a ray serves as the initial estimate for the solution along the next ray. The point on the boundary where the lowest value of Q is found is an estimate for x^* and the correspnding value of Q is an estimate for $Q(x^*)$.

Another approach has been followed in [1]. For a two-dimensional system in which the confidence contours are convex curves, exit was studied at the boundaries $x_1=0.1$ and $x_2=0.1$. Here, exit at $x_2=0.1$ is treated in detail. To obtain the point at $x_2=0.1$ which has the lowest Q-value the boundary conditions are formulated by

$$\begin{aligned} s\to-\infty: &\quad Q=0, \quad x_1=x_2=1 \text{ (the equilibrium)}, \\ s=0: &\quad x_2=0.1, \quad p_1=0. \end{aligned} \tag{3.28}$$

The condition $p_1=\partial Q/\partial x_1=0$ indicates that we are looking for an extremum of Q as a function of x_1. The initial estimate to the solution is a ray constructed by the initial value method which is believed to be close to the desired ray. Alternatively, first the problem is solved with $x_2=.9$ instead of 0.1. The solution of this problem is used as initial estimate to the solution of the problem with $x_2=.8$, etc. The procedure is repeated until the solution at $x_2=.1$ has been obtained. The boundary $x_1=0.1$ is treated in the same way. The boundary which contains the lowest value of Q is the most probable exit boundary and the point on this boundary where the minimum value is attained is the most probable exit point.

4. The shooting method

Shooting methods, in which the initial point of a characteristic is manipulated systematically in order to obtain the desired characteristic, have been used by Ludwig [7] to find the most probable exit point for a problem with type a boundary (the boundary of the state space is a type c boundary, but the boundary at which exit was studied was taken in the interior of the state space close to the boundary of the state space) and by H.E. de Swart and J. Grasman [9] to find the characteristic connecting equilibrium points in a stochastic model in meteorology. Results for these problems can be obtained easily by the boundary value method, while the use of shooting methods is rather elaborate because of the sensitivity to the choice of the initial point of the characteristic.

5. Intersecting rays

Rays starting in the neighbourhood of the equilibrium of a system of ray equations, with initial values chosen in accordance with the local analysis, may intersect. This leads to non-uniqueness of $Q(x)$. The global existence and uniqueness of solutions of ray equations is an important question which needs further theoretical investigation. In this section we confine ourselves to some remarks and a simple example.

In the one-dimensional stochastic system of example 1 the line introduced by the local analysis was tangent to the unstable manifold of the system of ray equations (1.6 ab) at the equilibrium point (in fact, both are coincident in the x,p-space). Also in the two-dimensional system of example 2 it is easily verified that the plane (3.27), following from the local analysis, is tangent to the unstable manifold at the equilibrium. Generally we have the following

Theorem. *The plane $p=Px$ in the x,p-space with P satisfying equation (2.4) is tangent to the unstable manifold of the system of ray equations (1.6 ab) at the equilibrium $x=p=0$.*

Proof. It is shown that the linearized unstable manifold at $x=p=0$ satisfies equation (2.4). Let the eigenvalues of B be given by λ_i $(i=1,2,\ldots,n)$. By the assumption of a stable deterministic equilibrium the real parts of the λ_i are negative. The eigenvalues of the system (3.10), which is the linearization of the system (1.6 ab) at $x=p=0$, are given by the λ_i with the corresponding eigenvectors $(w_i^t,0^t)^t$ and $-\lambda_i$ with the corresponding eigenvectors $(v_i^t,z_i^t)^t$, $i=1,2,\ldots,n$. Let $V=(v_1,v_2,\ldots,v_n)$, $Z=(z_1,z_2,\ldots,z_n)$ and L be the diagonal matrix containing $\lambda_1,\lambda_2,\ldots,\lambda_n$.

With respect to the eigenvalues $-\lambda_i$ corresponding to the unstable manifold we have by the definition of eigenvalues/vectors:

$$BV + AZ = -VL\,, \qquad (5.1)$$
$$-B^t Z = -ZL\,.$$

The unstable manifold is given by

$$\begin{bmatrix} x \\ p \end{bmatrix} = \sum_{i=1}^{n} \alpha_i \begin{bmatrix} v_i \\ z_i \end{bmatrix}, \qquad (5.2)$$

in which generally the parameters α_i and the elements of v_i and z_i are complex numbers. The last n equations in (5.2) are used to eliminate the α_i:

$$\alpha = Z^{-1} p\,, \qquad (5.3)$$

in which α is the vecor $(\alpha_1, \alpha_2, \ldots, \alpha_n)^t$. Substitution in the first n equations in (5.2) gives:

$$x = VZ^{-1} p \qquad (5.4)$$

and, by inversion,

$$p = ZV^{-1} x\,. \qquad (5.5)$$

This is the equation for the unstable manifold of the system (1.6 ab) at the equilibrium point. With the equations (5.1) it is easily shown that ZV^{-1} satisfies the equation (2.4) for P. So ZV^{-1} equals P.

In the example 1 the unstable manifold is $p = x - 1$, which is a single-valued function of x. For an n-dimensional stochastic system the characteristics, with initial values according to the local analysis, lie (approximately) on an n-dimensional hypersurface through the equilibrium point in the $2n$-dimensional x,p-space. On this hypersurface the characteristics do not intersect. From results in [6, 10] which exhibit non-uniqueness in $Q(x)$, we conclude that apparently this hypersurface may be folded so that the projections of the characteristics on the x-space (the rays) do intersect. Regions in the x-space where Q is non-unique are bounded by caustics. Caustic points can be detected numerically at the cost of a large amount of extra computation by keeping up the value of a Jacobian along the rays [6, 10].

A demonstration of non-uniqueness is given in the following example.

EXAMPLE 3.
Consider the two-dimensional system

$$\left.\begin{aligned} b_1(x) &= x_1(1-x_1) + x_2\,, \\ b_2(x) &= -\beta x_2\,, \qquad (\beta > 0, \neq 1) \\ a_1(x) &= 1\,, \\ a_2(x) &= 1\,. \end{aligned}\right\} \qquad (5.6)$$

The deterministic system has the equilibrium points $x_1 = 0$, $x_2 = 0$ and $x_1 = 1$, $x_1 = 0$. The latter equilibrium is stable. A WKB-Ansatz leads to the ray equations:

$$\left.\begin{aligned} \frac{dx_1}{ds} &= x_1(1-x_1) + x_2 + p_1\,, \\ \frac{dx_2}{ds} &= -\beta x_2 + p_2\,, \end{aligned}\right\} \qquad (5.7a)$$

$$\left.\begin{aligned} \frac{dp_1}{ds} &= (2x_1 - 1)p_1\,, \\ \frac{dp_2}{ds} &= -p_1 + \beta p_2\,, \end{aligned}\right\} \qquad (5.7b)$$

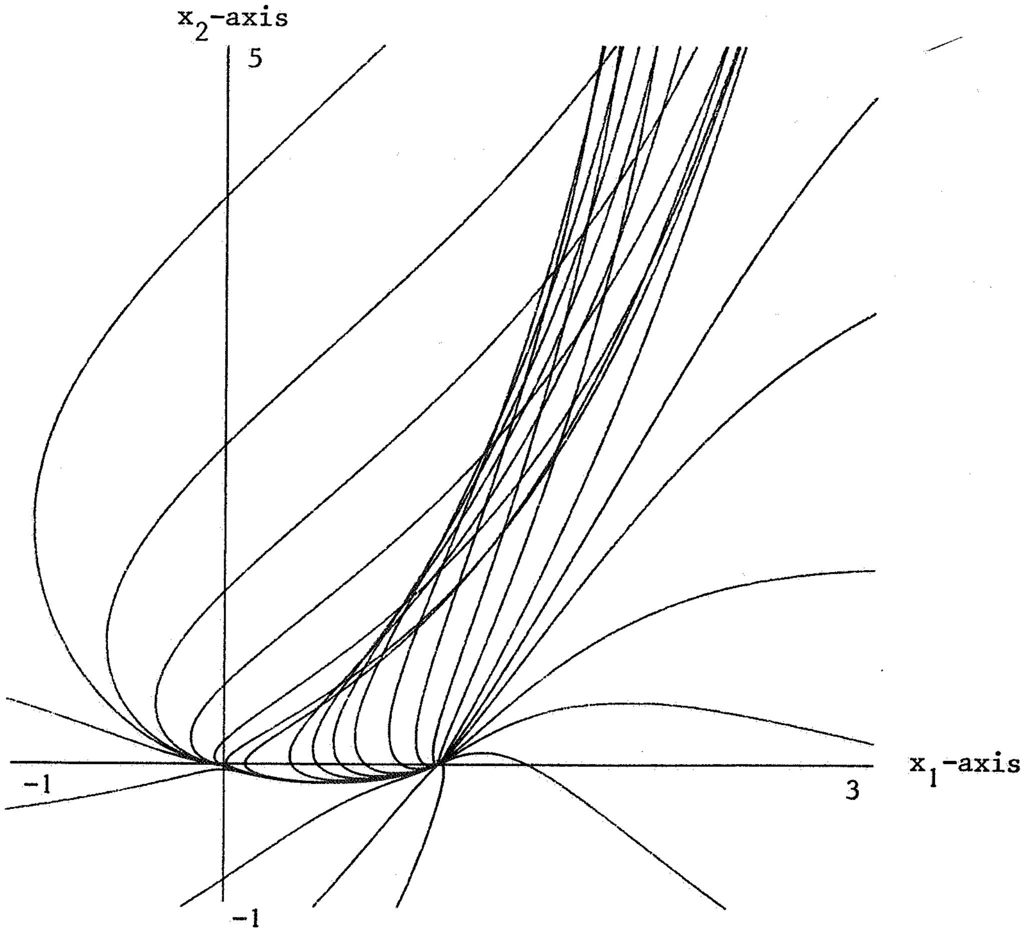

FIGURE 5. Demonstration of intersecting rays.

$$\frac{dQ}{ds} = \frac{1}{2}(p_1^2 + p_2^2)\,. \tag{5.7c}$$

The system (5.7 ab) has the equilibrium points

$$\left[\frac{1}{2}, \frac{-1}{4(1+\beta^2)}, \frac{-\beta^2}{4(1+\beta^2)}, \frac{-\beta}{4(1+\beta^2)}\right]^t, \tag{5.8}$$

$$(0,0,0,0)^t\,,$$

$$(1,0,0,0)^t\,.$$

The matrix P, following from the local analysis is given by

$$P = \frac{2(1+\beta)}{\beta^2+2\beta+2}\begin{bmatrix} 1+\beta & -1 \\ -1 & \beta^2+\beta+1 \end{bmatrix}. \tag{5.9}$$

The system (5.7) has been solved numerically by the initial value method, in which the initial points were chosen on a circle with radius .01 around $x_1=1$, $x_2=0$ and the corresponding values of p_1, p_2 and Q were chosen according to the local analysis. Fig. 5 shows rays for $\beta=3/2$. A number of rays were chosen very close to the ray connecting $x_1=1$, $x_2=0$ with $x_1=0$, $x_2=0$. In the neighbourhood of $x_1=0$, $x_2=0$ part of those rays turn away to the right and intersect other rays. The figure looks like the projection of a cusp manifold. In the region in the x-space between the caustics (the projection of the 'cusp edges') $Q(x)$ is a 3-valued function. It is not clear whether the non-uniqueness is genuine or due to finite precision arithmetic c.f. the remark corresponding to example 1.

6. Reformulation of the boundary value method

The boundary value method can be reformulated as follows:

$s \to -\infty$: *i)* $Q=0$

ii) x and p must lie on the plane tangent the unstable manifold at the equilibrium $x=p=0$. (6.1)

$s=0$: $x=e$

The condition ii) leads to n linear relations between elements of x and p. See example 2 and the theorem in section 5. In a mathematical sense this formulation is better than the formulation (3.1). From the practical point of view the formulation (3.1), if applicable, is preferable to the formulation (6.1), because it doesn't require the computation of the eigenvalues/vectors to determine the unstable manifold at $x=p=0$.

7. Discussion

In this technical note we discussed the initial value method, the boundary value method and the shooting method in relation to the solution of certain problems in stochastic systems described by the ray equations. The initial value method is the most appropriate method in the case that one is interested in the construction of a ray starting from a point at which the values of x,p and Q are known. Numerical integration routines for initial value problems exist, by which the solution can be obtained with a high accuracy.

The boundary value method is a convenient method to construct a characteristic which has a specific point x as its endpoint. The numerical integration routine for boundary value problems, which has been discussed in this technical note, needs a good initial estimate in order to iterate to the solution. The initial estimate can be based on the known values of x,p and Q along a neighbouring characteristic. The accuracy of the numerical results with the boundary value method is not as high as the accuracy of the numerical results with the initial value method, but it is possible that a higher accuracy still can be achieved by optimizing the numerical procedure, for example by making the interval between the grid points s variable, depending on the gradients of certain variables, or by using a larger number of grid points. For the present purposes, see [1], the accuracy was considered sufficient. In this technical note various examples have been given in which the boundary value method proved to be a convenient tool, specifically in the construction of confidence contours and in the construction of characteristics connecting equilibria (heteroclinic trajectories). A variety of other applications of the initial value method and the boundary value method is conceivable, for example the construction of a characteristic *through* a specific point x.

A few purposes have been mentioned in which the shooting method was applied. In those cases results are obtained in a less elaborate way by the boundary value method. The shooting method should be used only in cases that a high accuracy is required.

The ray method may lead to a non-unique solution of Q in regions of the x-space. This should be kept in mind when the methods described in this technical note are used.

ACKNOWLEDGEMENTS

I want to thank Johan Grasman and Huib de Swart for remarks on the text and/or discussions.

REFERENCES

[1] ROOZEN, H. *Equilibrium and extinction in stochastic population dynamics.* Report AM-R8602, Centre for Mathematics and Computer Science, Amsterdam, 1986.

[2] MATKOWSKY, B.J. and Z. SCHUSS. *The exit problem for randomly perturbed dynamical systems.* SIAM J. Appl. Math. Vol. 33, No. 2, 1977.

[3] MATKOWSKY, B.J. and Z. SCHUSS. *Diffusion across characteristic boundaries.* SIAM. J. Appl. Math. Vol. 42, No. 4, 1982.

[4] MATKOWSKY, B.J., Z. SCHUSS and C. TIER. *Diffusion across characteristic boundaries with critical points.* SIAM. J. Appl. Math. Vol. 43, No. 4, 1983.

[5] HANSON, F.B. and C. TIER. *An asymptotic solution to the first passage problem for singular diffusion in population biology.* SIAM. J. Appl. Math. Vol. 40, No. 1,1981.

[6] LUDWIG, D. *Persistence of dynamical systems under random perturbations.* SIAM. Review Vol. 17, No. 4, 1975.

[7] NAG- library, Fortran. *Numerical Algorithms group.* Mayfield House, 256 Banbury Road, Oxford 0X2 7DE, United Kingdom.

[8] FELLER, W. *The parabolic differential equations and the associated semigroups of transformations.* Ann. Math. 55: 468-519, 1952.

[9] DE SWART, H.E. and J. GRASMAN. *Effect of stochastic perturbations on a spectral model of the atmospheric circulation.* Report AM-R8515, Centre for Mathematics and Computer Science, Amsterdam, 1985.

[10] LANKELMA, J.V. *Stochastic dynamical systems with a cyclic structure.* Report TW 247/83, Centre for Mathematics and Computer Science, Amsterdam, 1983.