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THIRD AUTUMN WORKSHOP ON MATHEMATICAL ECOLOGY

(14 October - 1 November 1996)

"Physiological Ecotoxicology: Mathematical Theory and Simulation Applications"

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PHYSIOLOGICAL ECOTOXICOLOGY: MATHEMATICAL THEORY AND SIMULATION APPLICATIONS

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OUTLINE

1. STRESSOR ECOLOGY
   - PHYSICAL
   - CHEMICAL
   - BIOLOGICAL
2. PROTOCOL: MODELS FOR ASSESSMENT
   - INDIVIDUAL
     - PHYSIOLOGICAL
     - STRESSOR EXPOSURE
     - EFFECTS
   - POPULATION
     - STRESSED DYNAMICS
   - RESOURCE - CONSUMER COMMUNITY
     - SPATIAL DYNAMICS
     - STRESSED DYNAMICS

COAUTHORS: RAY LASSITER, GRACIELA CANZIANI, SHANDELLE HENSON, ERIC FUNASAKI, DINA LIKA, HOCK LYE KOH, H L LEE AND PROBABLY 15 MORE.

STRESSOR ECOLOGY FOR AQUATIC SYSTEMS

1. PHYSICAL STRESSORS
   (Temperature, dissolved oxygen, salinity, pH...)

   - EXPOSURE
     - VARIABILITY
   - EFFECTS

2. CHEMICAL STRESSORS
   (Organics, metals, ...)

   - EXPOSURE
   - EFFECTS

STRESSOR EXPOSURE AND EFFECTS

EXPOSURE

- CHARACTERISTICS OF RECEPTOR ARE IMPORTANT
  - LIPIDS - lipophilic chemicals
  - CELL WALLS - heavy metals
  - metabolic pathways

EFFECTS

- STRESSORS AFFECT PHYSIOLOGICAL PROCESSES AND BEHAVIOR
- ADAPTATIVE PROTECTION AGAINST STRESS

POPULATION LEVEL EFFECTS

TEMPORAL DYNAMICS

- TRANSCIENT
- ASYMPTOTICS
- RETROSPECTIVE - INVERSE APPROACH

STRESSED COMMUNITY DYNAMICS

- RESOURCE - CONSUMER SYSTEM
  - SPATIAL
  - LETHAL EFFECTS
- MATHEMATICS
  - TRAVELING WAVES

Methodology

The protocol used to study the effects of chemicals on a fish population utilizes the following components:

- individual model
- toxicant exposure and effect models
- population model coupling temporal–spatial processes with physiological processes of individuals and a dynamic resource.

Individual Model

(Hallam et al. (1996))

$$\frac{dm_l}{dt} = g_l(m_l, m_s, X) = \frac{a_{0l}X_l}{X}F - a_1(m_l - \epsilon m_{ps})\frac{E_d}{E_a}$$

$$\frac{dm_s}{dt} = g_s(m_l, m_s, X) = \frac{a_{0s}X_s}{X}F - a_2(m_s - m_{ps})\frac{E_d}{E_a}$$

X	density of resource (g/cm^3)
X_l	density of resource lipid (g/cm^3)
X_s	density of resource structure (g/cm^3)
a_{0l}	lipid assimilation efficiency
a_{0s}	structure assimilation efficiency
F	feeding rate (g/d)

$$E_a = 3.786 \times 10^4 a_1(m_l - \epsilon m_{ps}) + 1.675 \times 10^4 a_2(m_p - m_{ps})$$

$E_d =$ maintenance + specific dynamic action
activity + reproduction

Predator-prey model

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho}{\partial a} + \frac{\partial (g_l\, \rho)}{\partial m_l} + \frac{\partial (g_s\, \rho)}{\partial m_s} + \frac{\partial (q\rho)}{\partial x} = -\mu\rho$$

$$\frac{dr}{dt} = \alpha\, r(1 - \frac{r}{K}) - \int_0^\infty\int_0^\infty\int_0^\infty F\ \rho\ da\ dm_l\ dm_s$$

$\rho(t, a, m_l, m_s, x)$	fish density
$r(t, x)$	resource density
$g_l = g_l(m_l, m_s, X)$	growth rate of m_l
$g_s = g_s(m_l, m_s, X)$	growth rate of m_s
$q = q(m_l, m_s, x)$	movement rate of an individual
α	growth rate of the resource
K	carrying capacity
$F = F(m_l, m_s, X)$	feeding rate (g/d)

$$\rho(0, a, m_l, m_s, x) = \rho_0(a, m_l, m_p, x)$$

$$r(0, x) = r_0(x)$$

$$q\rho = 0 \text{ on } \partial\Omega$$

$$\rho(t, 0, m_{l0}, m_{s0}, x) = \int_0^\infty\int_0^\infty\int_0^\infty \beta\ \rho\ da\ dm_l\ dm_s$$

Spatial movement

$$q = \kappa v_s \frac{\partial r}{\partial x}$$

$$q = \begin{cases} 0 & if\ \ E_g > E_d \\ \kappa v_s \frac{\partial r}{\partial x} & if\ \ E_g \le E_d \end{cases}$$

$$v_s \sim sL$$

$r(t, x)$	resource density
κ	distance covered by a foraging fish per unit change in the prey density
v_s	average swimming velocity
s	body length per sec of a fish while cruising
E_g	energy gained
E_d	energy demands

Reproduction

- periodic reproduction ($T = 365$)
- $\beta = \beta(m_l, m_s)$

Mortality

- age-dependent mortality
- juvenile density-dependent mortality
- maximum age
- starvation

Uptake model

(Lassiter et al. (1990))

Modification of FGETS (Barber et al. (1988))

$$\frac{dC_T}{dt} = k_1 C_w + \frac{F}{W_T} C_F - k_2 C_T - \frac{E k_E}{W_T} C_A - \frac{1}{V}\frac{dV}{dt} C_T$$

C_T	Toxicant concentration in whole fish
C_w	Toxicant concentration in ambient water
C_A	Toxicant concentration in aqueous portion of the fish
C_F	Toxicant concentration in intestinal contents
F	Weight of ingested food per day
E	Weight of material defecated per day
k_E	Partition coefficient of chemical to excrement
V	Volume of the organism
W_T	Weight of the organism
k_1	Uptake rate of the environmental chemical
k_2	Depuration rate of the environmental chemical

$$k_1 = S_g k_w V^{-1}$$

$$k_2 = S_g k_w V^{-1}(P_A + P_L K_L + P_S K_S)^{-1}$$

S_g	Active exposure area
P_A	Fraction of fish that is aqueous
P_L	Fraction of fish that is lipid
P_S	Fraction of fish that is structure
k_w	Conductivity:exposure
K_L	Lipid/water partition coefficient
K_S	Structure/water partition coefficient

$$C_T = (P_A + P_L K_L + P_S K_S) C_A$$

C_T	Toxicant concentration in whole fish
C_A	Toxicant concentration in aqueous portion of the fish
P_A	Fraction of fish that is aqueous
P_L	Fraction of fish that is lipid
P_S	Fraction of fish that is structure
K_L	Lipid/water partition coefficient
K_S	Structure/water partition coefficient

Effects of toxicants

- mortality

$$\log LC_{50} = -0.8 - \log K_{ow}$$

LC_{50} Lethal concentration
K_{ow} octanol/water partition coefficient

(Veith et al. (1983) and Konemann (1981))

Prey–Directed Movement for a Structured Fish Population

Lethal Effects of Toxicants on the Fish Population

Results

Unstressed System: Continuous movement

Total fish and resource biomass, as well as age, lipid, and structural distributions of the fish population exhibit asymptotically periodic behavior for parameter values that result in the coexistence of the two populations.

Through the energetic cost of swimming and feeding rate the characteristic velocity, s, of the population affects the growth of individuals in a counteractive way.
Consequently, the population dynamics are also affected by s. There is an optimal value for s that maximizes the fish biomass.

Continuous movement vs. movement based on energetic constraints

For low values of s, continuous movement is better than the movement based on energetic constraints.
For large values of s, continuous movement is not favorable to the individuals.

Results

Stressed System: Continuous movement

Spatial heterogeneity can influence the physiological structure of the population and determine the survival or extinction of the population. These depend on the spatial pattern of the toxicant and resource, as related to the distribution of individuals in space, during the exposure.

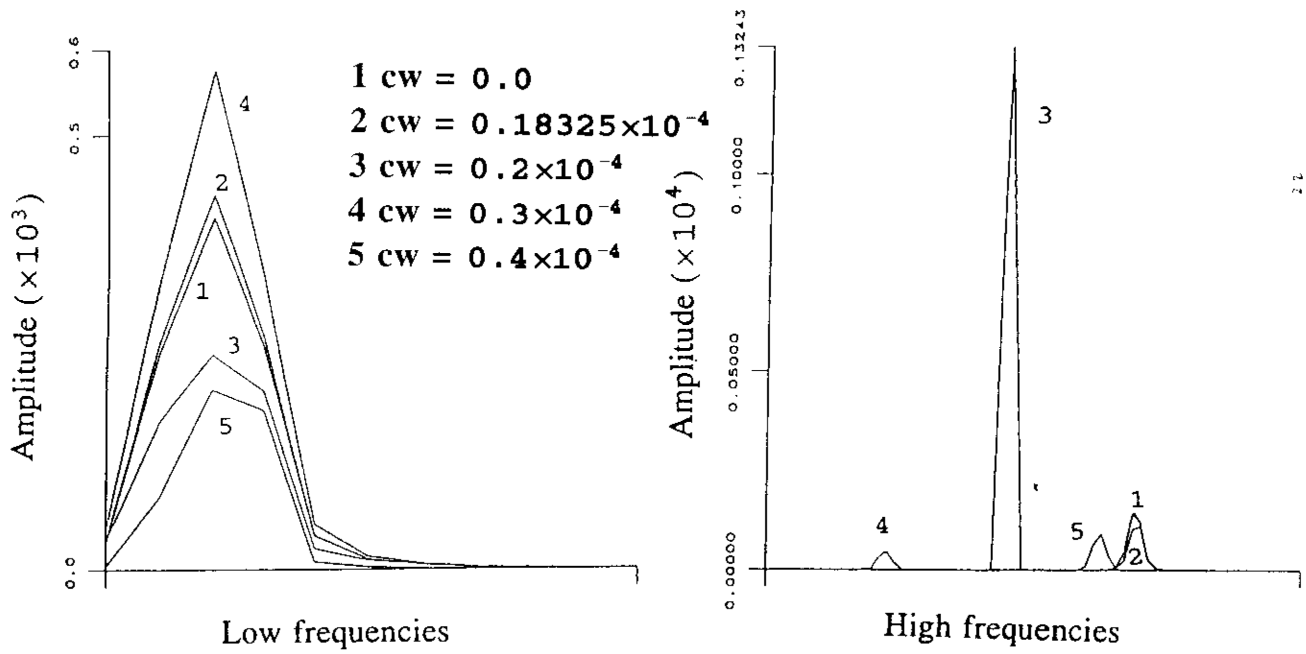
The spatial pattern of the toxicant and resource, as related to the distribution of individuals in time and space, can influence the structure of the population.

The theory of the survival of the fattest (Lassiter and Hallam (1990))

- static population
- homogeneous toxic exposures

Frequency Analysis (work by Dina Lika)

Fast Hartley Transform was used to construct the power spectrum of time-series data from the Daphnia population model. No indicator could be found as chemical concentration was varied. (Value of *cw*)



PART II.

MAIN OBJECTIVES:

- ***DISCUSSION OF TRANSIENT DYNAMICS FOR SUBLETHALLY STRESSED POPULATIONS***
- ***SIMPLE STRESS INDICATORS FROM POPULATION SUMMARY STATISTICS***

TRANSIENT DYNAMICS:

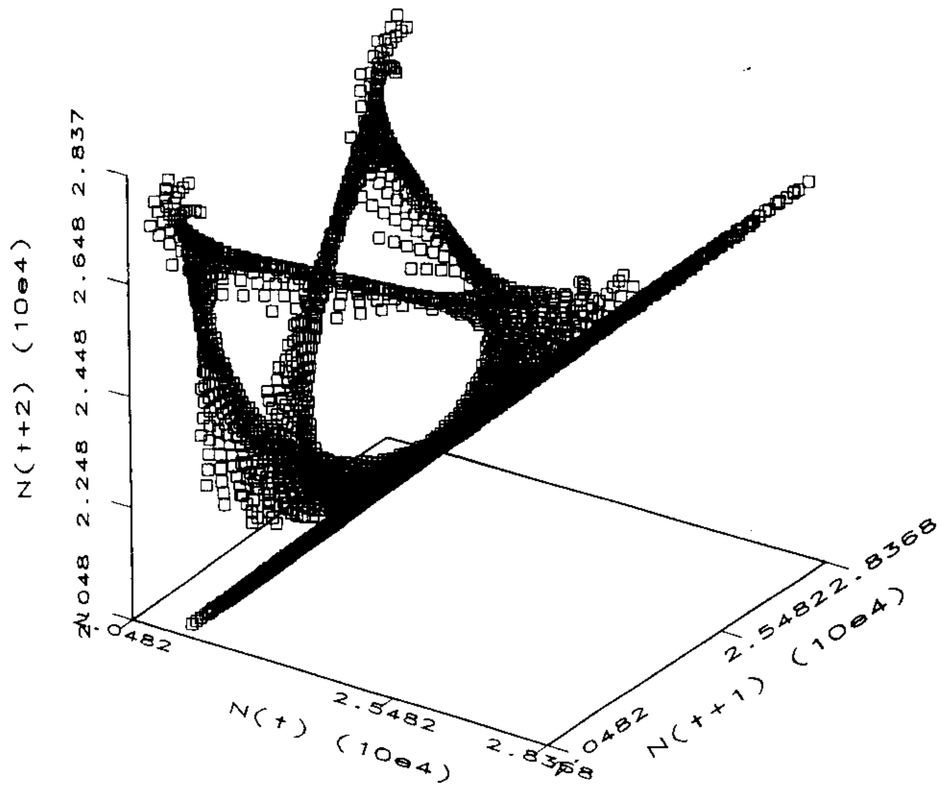
E. Funasaki and T. G. Hallam, manuscript in preparation on long temporal behavior of dynamics.

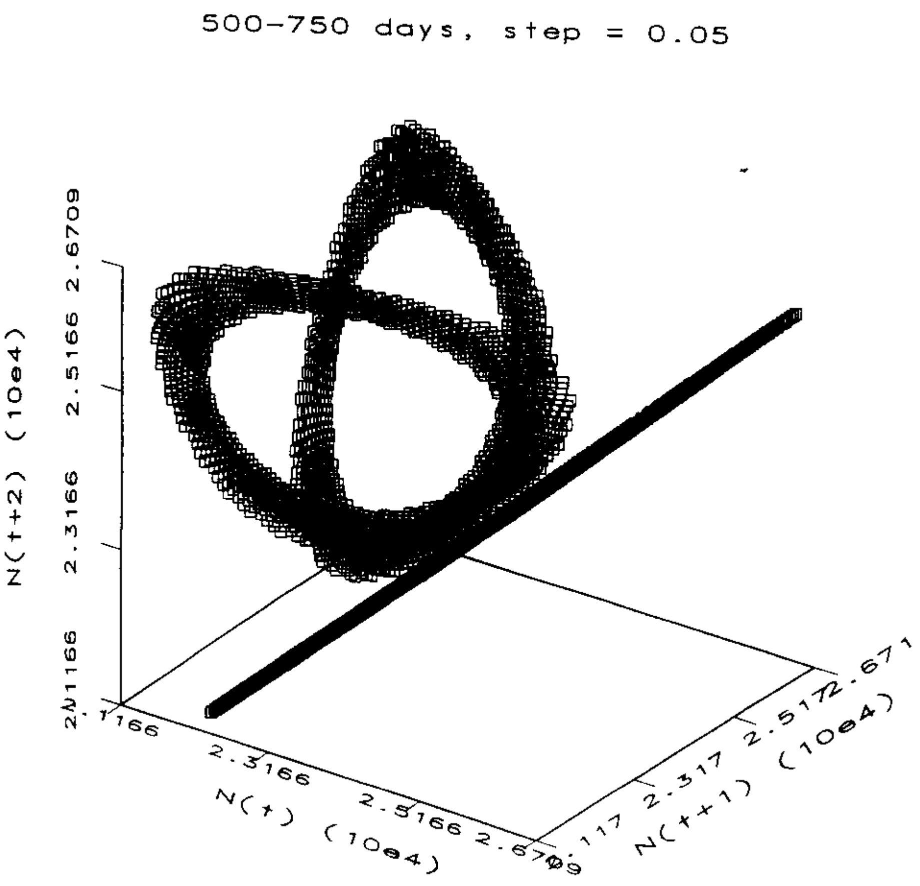
A. Hastings and Higgens, Science.

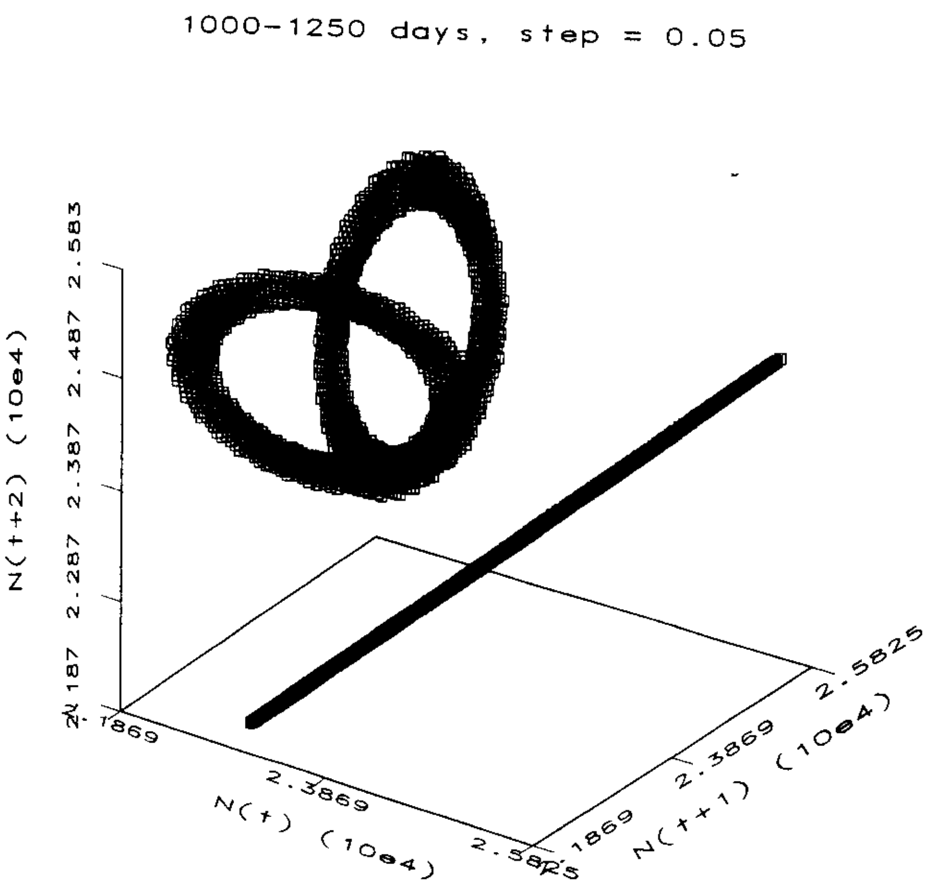
D. Lika, dissertation

uses only single ecotype

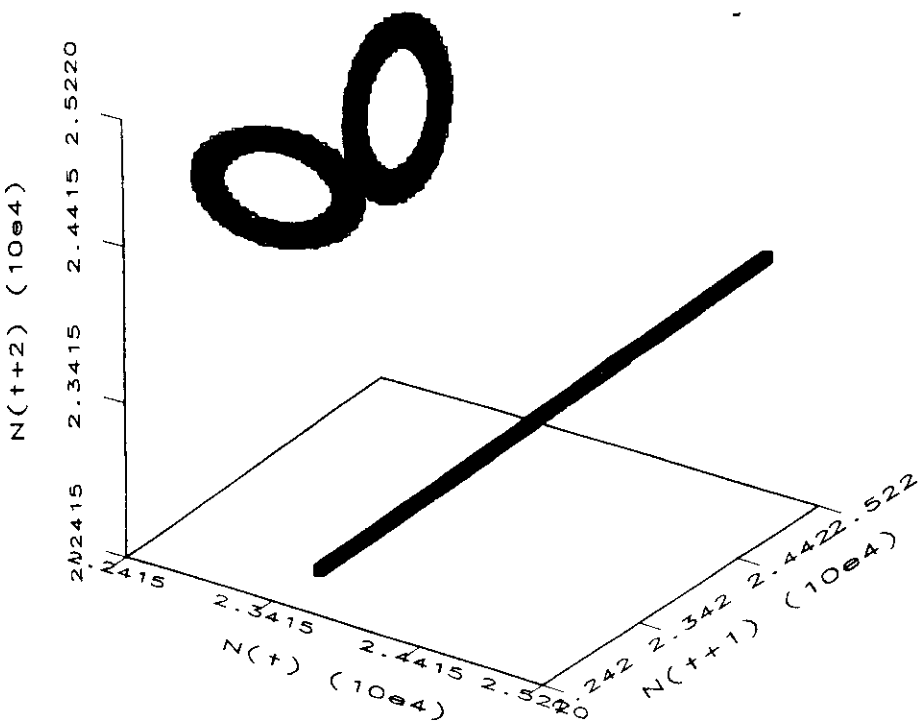
250–500 days, step = 0.05



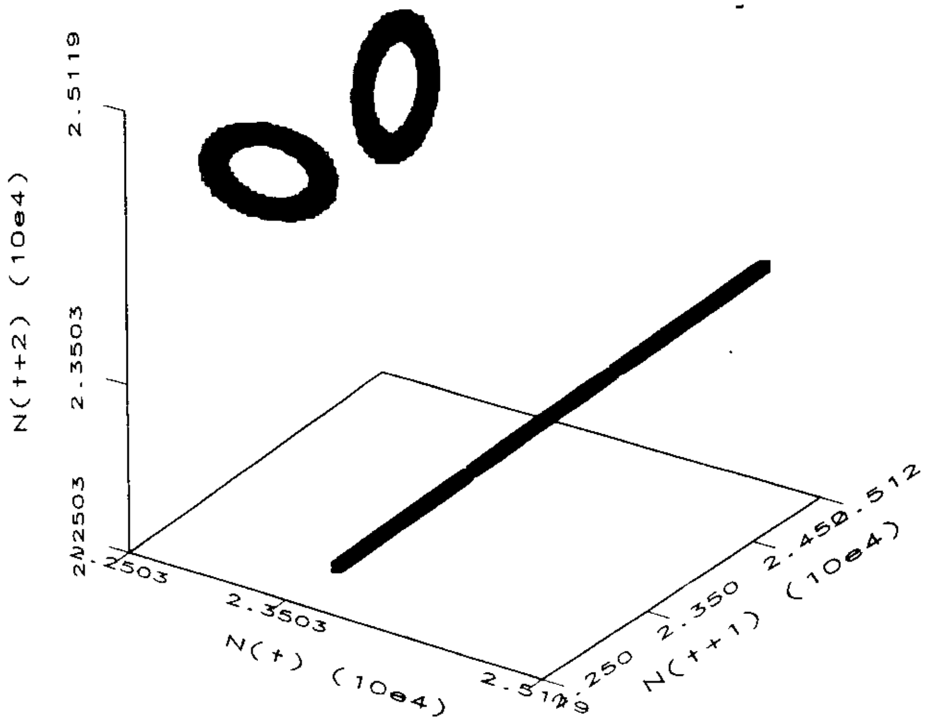

500-750 days, step = 0.05
N(t+2) (10e4)
2.1166
2.3166
2.5166
2.6709
N(t) (10e4)
2.3166
2.5166
N(t+1) (10e4)
2.317
2.517
2.671


1000-1250 days, step = 0.05
N(t+2) (10e4)
2.187
2.287
2.387
2.487
2.583
N(t) (10e4)
2.1869
2.3869
N(t+1) (10e4)
2.3869
2.5825

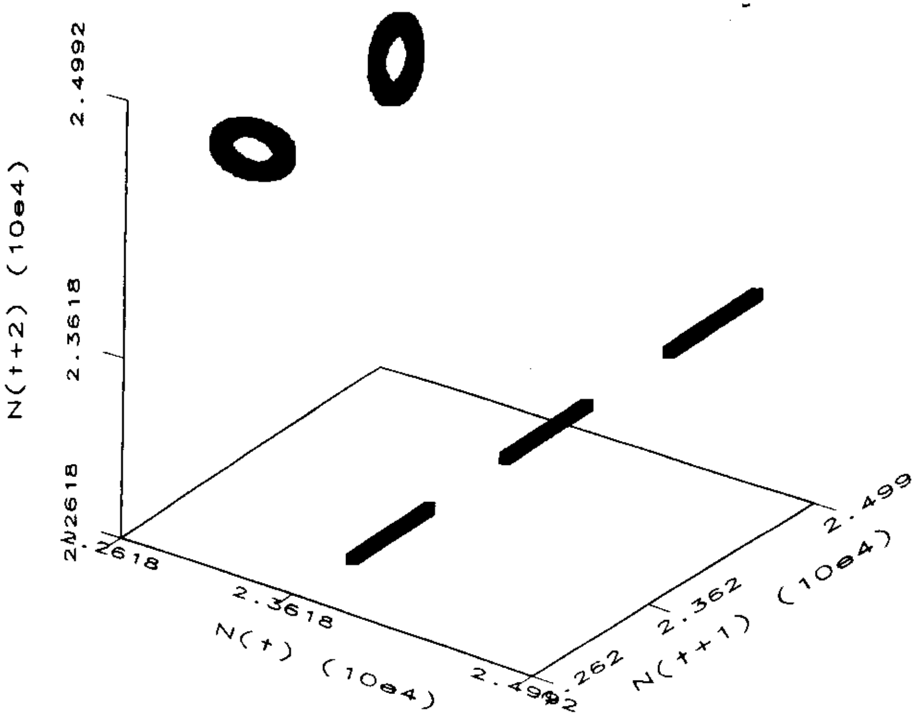
1750-2000 days, step = 0.05



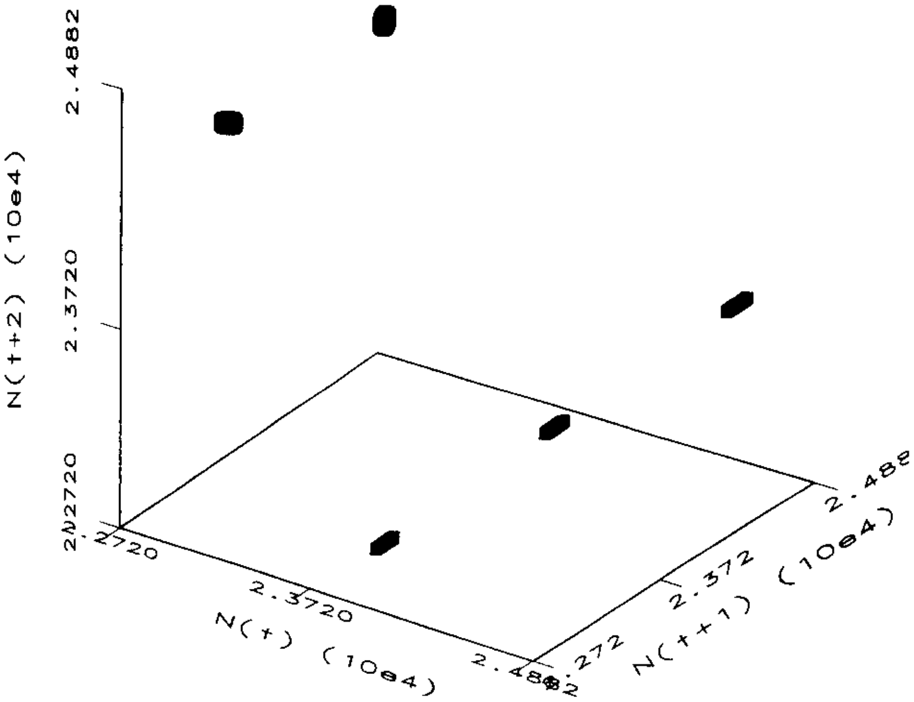
2000-2250 days, step = 0.05

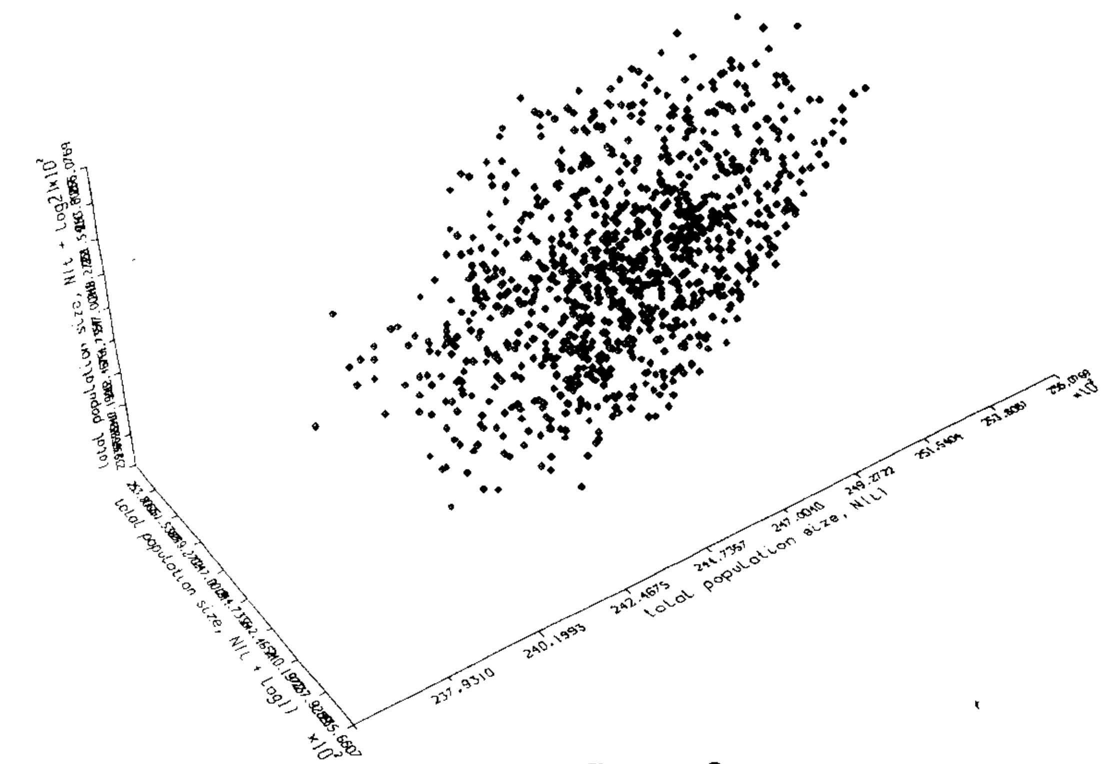


2500–2750 days, step = 0.05

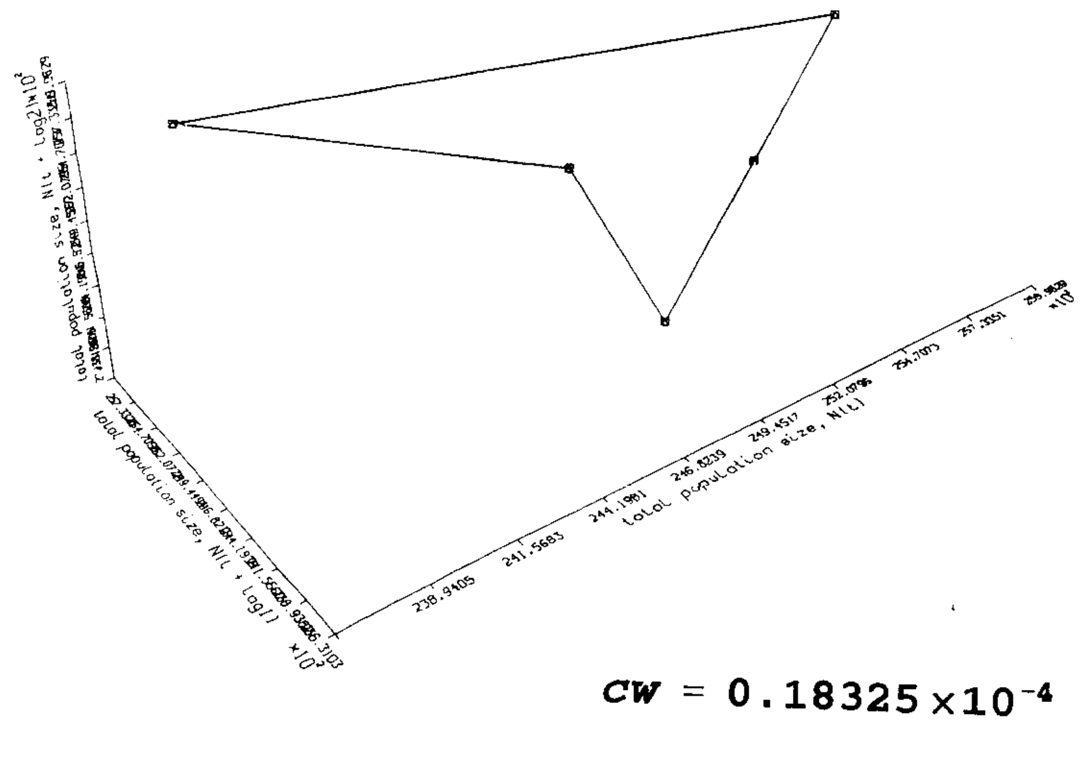


3750–4000 days, step = 0.05

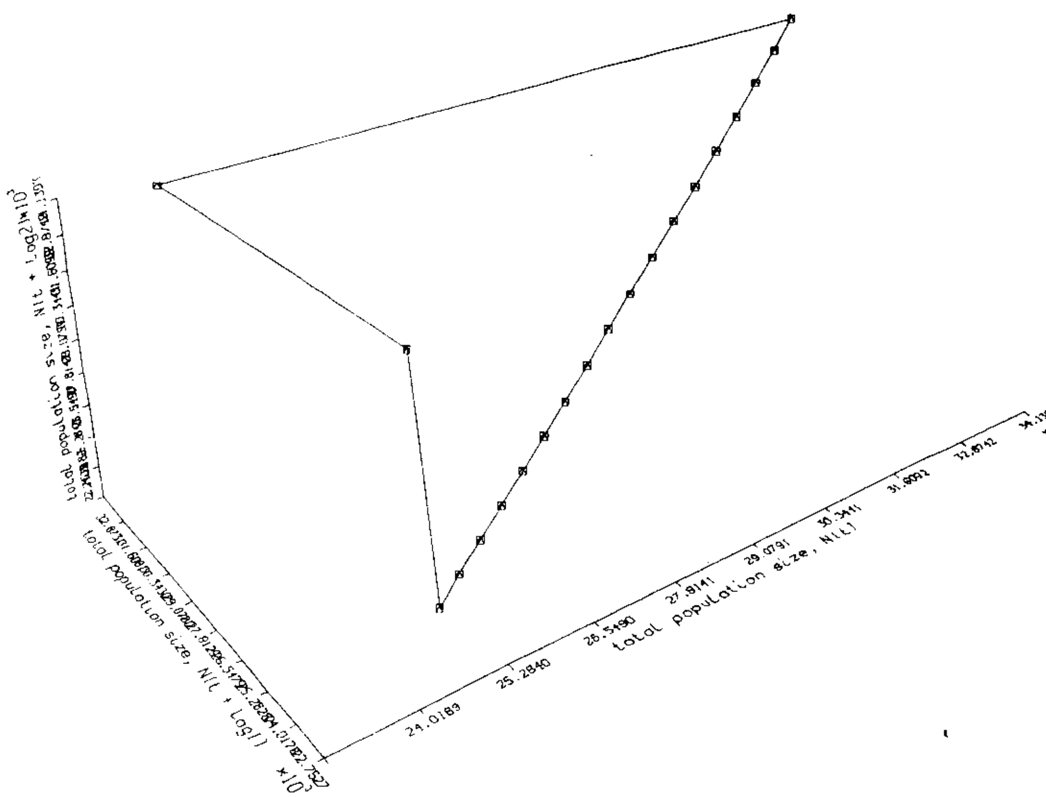




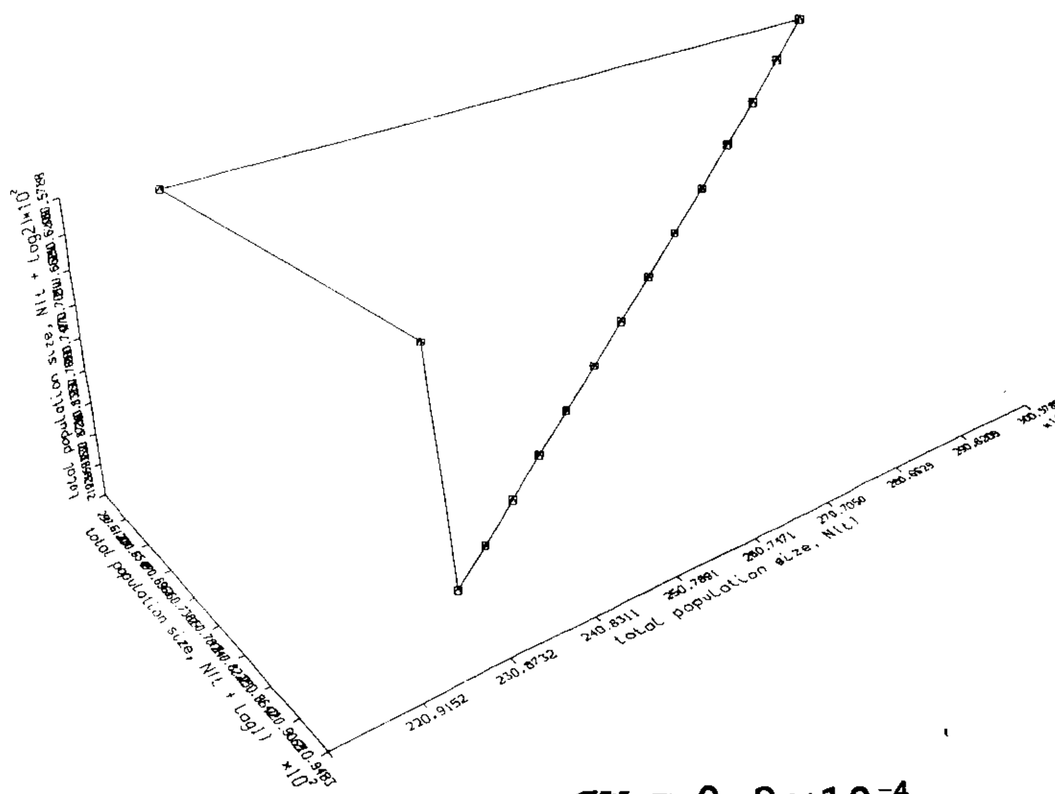
$CW = 0.1833 \times 10^{-4}$



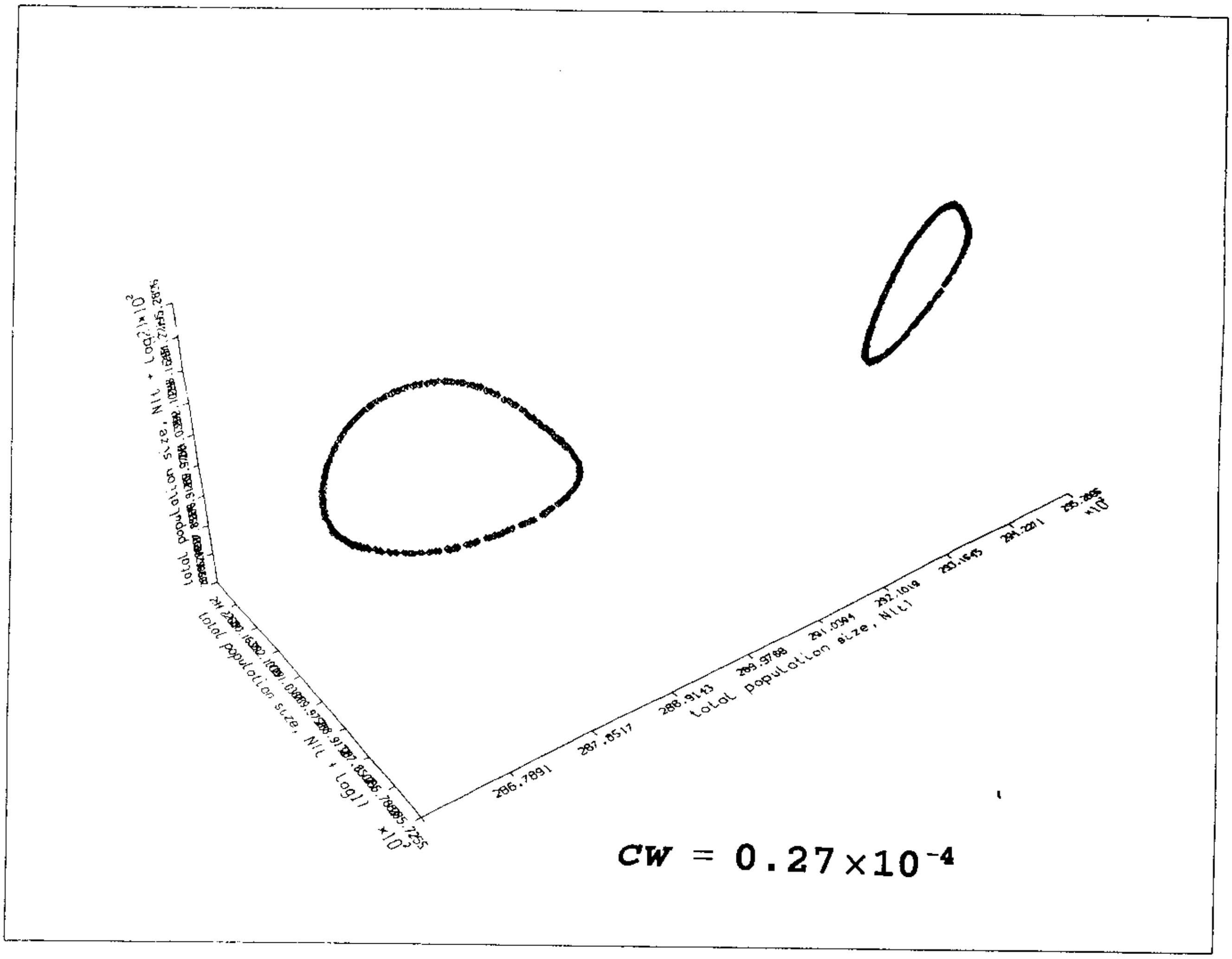
$CW = 0.18325 \times 10^{-4}$



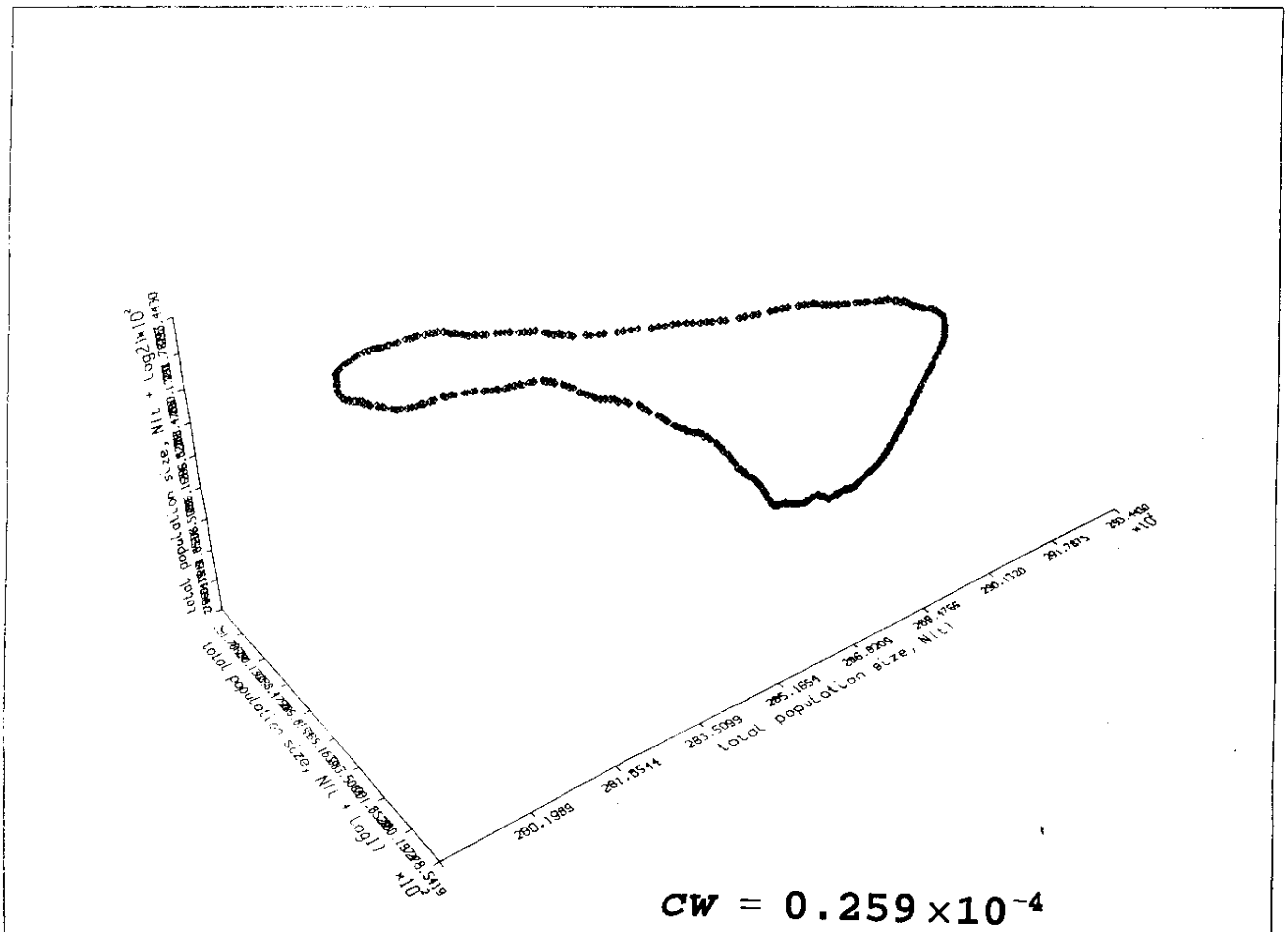
$CW = 0.257 \times 10^{-4}$



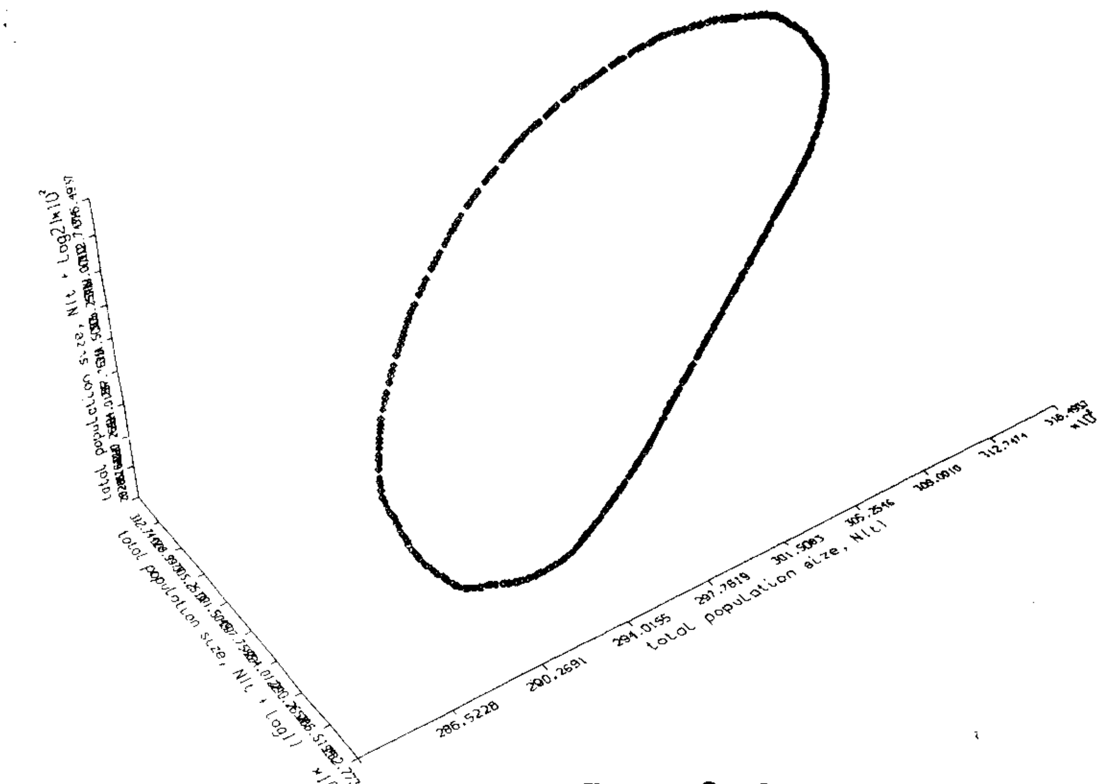
$CW = 0.2 \times 10^{-4}$



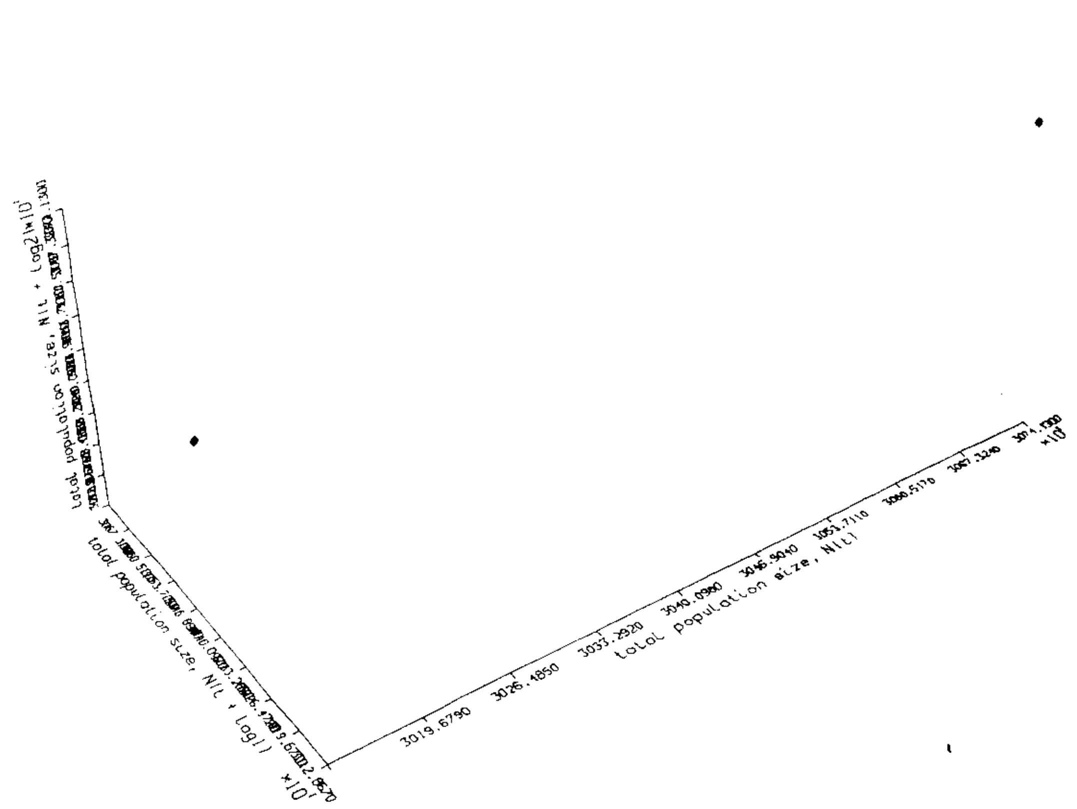
total population size, N(t)
$CW = 0.27\times10^{-4}$



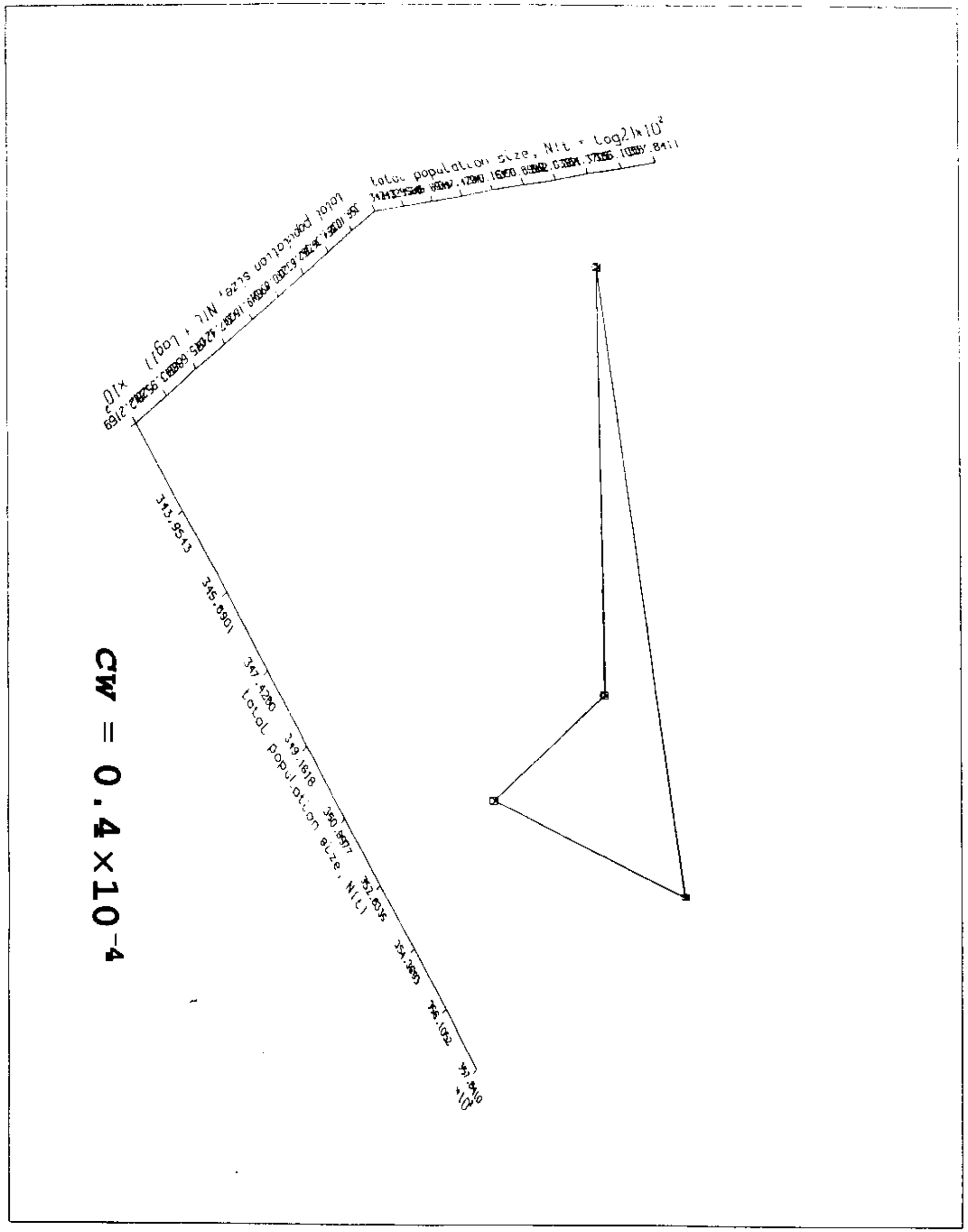
total population size, N(t)
$CW = 0.259\times10^{-4}$



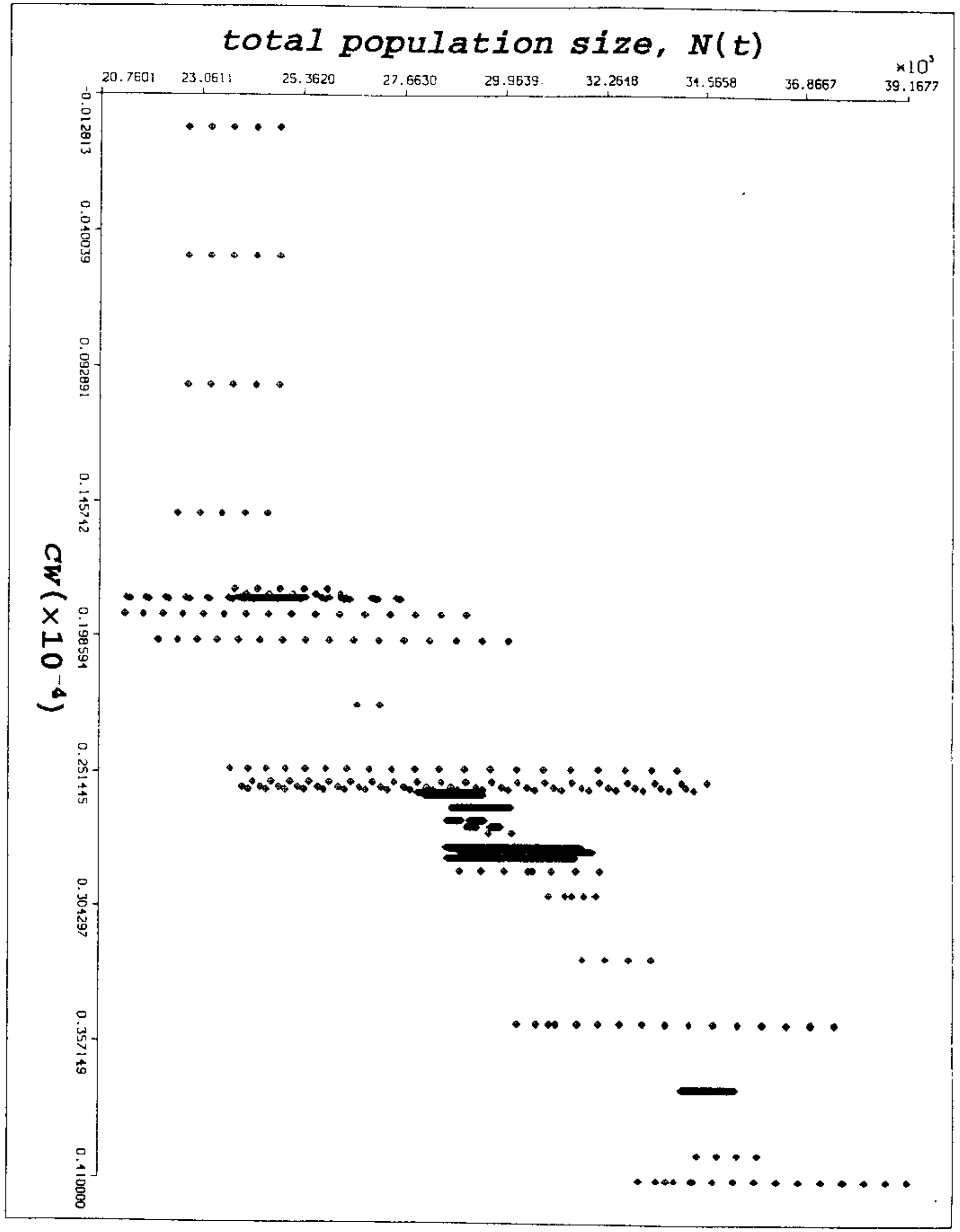
$CW = 0.2805 \times 10^{-4}$



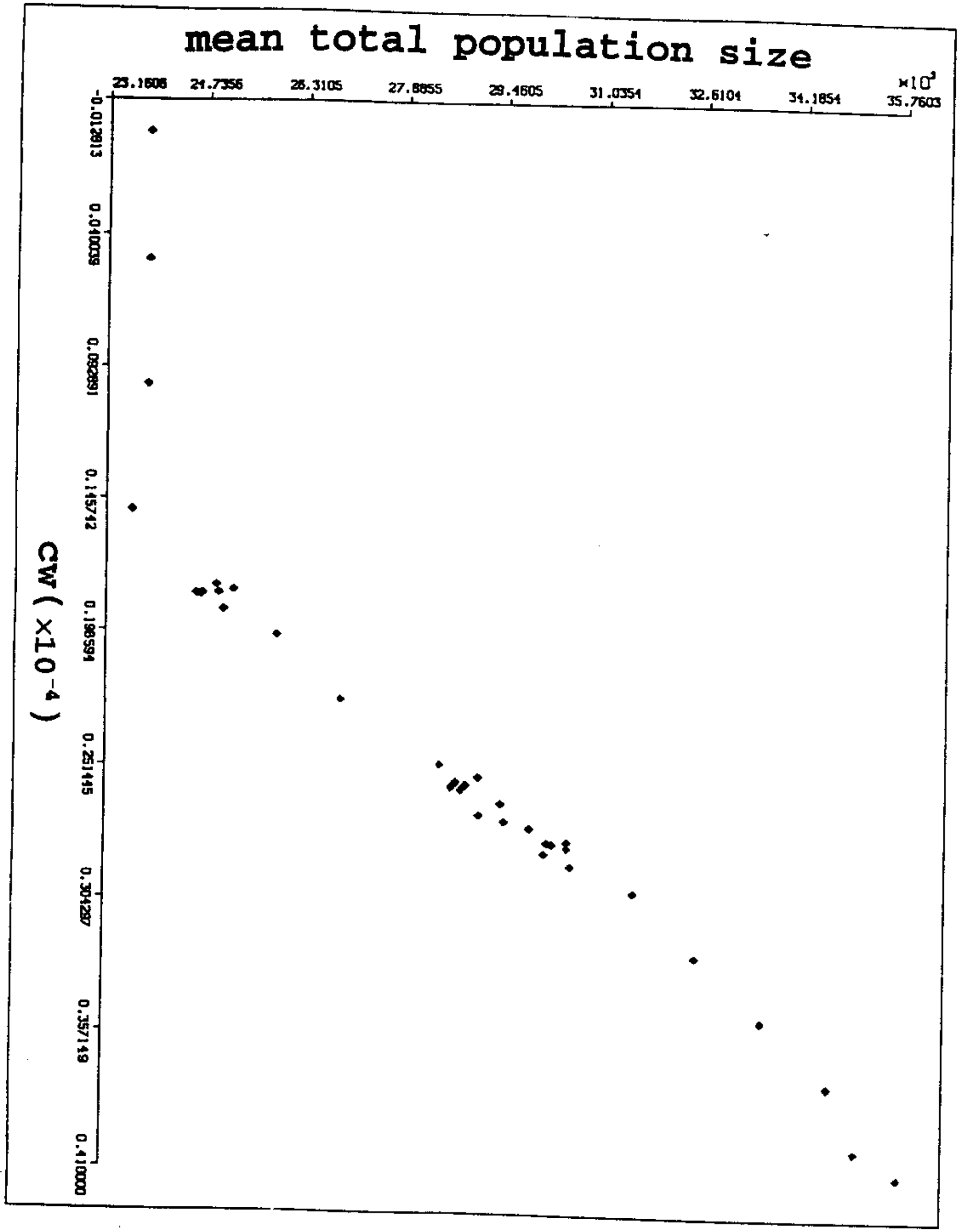
$CW = 0.28 \times 10^{-4}$



CW = 0.4×10-4
total population size, N(t)
total population size, N(t + log1)
total population size, N(t + log2)
343.9543
345.6901
347.4260
349.1618
350.8977
352.6335
354.3693
356.1052



total population size, N(t)
×10³
20.7601
23.0611
25.3620
27.6630
29.9639
32.2648
34.5658
36.8667
39.1677
CW(×10-4)
-0.012813
0.040039
0.092891
0.145742
0.198594
0.251445
0.304297
0.357149
0.410000



WHAT IS IMPORTANT FOR STRESSOR ECOLOGY?

- **Averages - biomass**
- **Population level parameters that change with stressors and stressor levels**
    - **Length of juvenile period - time to first birth.**

Should assessment scientists care about dynamics of ecological systems?

- **Dynamics are highly variable, not only in these models but in natural populations.**
- **Fluctuations do not appear predictable as stressors are changed.**
- **Scale is fundamental in that some systems are virtually nonreplicable.**

ANSWER: NO!

PART III

Predator–Prey Pursuit Model

$$(6)\qquad \begin{aligned} \frac{\partial N}{\partial t} &= rN\left(1-\frac{N}{K}\right) - \gamma NP \ , \\ \frac{\partial P}{\partial t} + k\frac{\partial}{\partial x}\left(P\frac{\partial N}{\partial x}\right) &= eNP - \mu P \ . \end{aligned}$$

We nondimensionalize the system by setting

$$U = \tfrac{N}{K} \ , \quad V = \tfrac{\gamma P}{r} \ , \quad t^* = rt \ ,$$
$$x^* = \sqrt{\tfrac{r}{kK}}\,x \ , \quad a = \tfrac{eK}{r} \ , \quad b = \tfrac{\mu}{eK} \ .$$

System (??) becomes

$$(7)\qquad \begin{aligned} \frac{\partial U}{\partial t} &= U(1-U-V) \ , \\ \frac{\partial V}{\partial t} + \frac{\partial}{\partial x}\left(V\frac{\partial U}{\partial x}\right) &= aV(U-b) \ , \end{aligned}$$

where a and b are positive constants.

Spatially Independent System

Steady Sta es:

$(0,0)$	:	saddle point,
$(1,0)$	:	saddle point,

$$(b, 1-b), \quad b<1 \; : \; \begin{cases} \text{stable node, if} & 4a \le b/(1-b), \\ \text{stable focus, if} & 4a > b/(1-b). \end{cases}$$

Traveling Wave Solutions

We look for solutions of the form

(8) $$U(x,t) = u(z), \quad V(x,t) = v(z), \quad z = x + ct.$$

Substituting (??) into (??), we obtain

(9) $$\begin{aligned} cu' &= u(1-u-v) \;\; , \\ cv' + (vu')' &= av(u-b) \;\; . \end{aligned}$$

$$(\mathrm{I}) \qquad \begin{aligned} u' &= \frac{1}{c}u(1-u-v) \ , \\ v' &= \frac{v}{c}\ \frac{ac^2(u-b) - u(1-u-v)(1-2u-v)}{c^2 + u(1-u-2v)} \ , \end{aligned}$$

for $(u, v) \notin S$, where

$$S = \{(u, v) \in R_+ \times R_+ \mid h(u, v) \equiv c^2 + u(1-u-2v) = 0\}$$

is the singularity set of the second equation in (I).

For $(u, v) \in S$, the vector field is described by the following system of equations

$$(\mathrm{II}) \qquad \begin{aligned} u' &= \frac{1}{2c}[u(1-u) - c^2] \ , \\ v' &= -\frac{u^2 + c^2}{4cu^2}[u(1-u) - c^2] \ . \end{aligned}$$

Isoclines for the system (I)

$$u = 0, \ v = 0,$$

$$f(u, v) \equiv 1 - u - v = 0,$$

$$g(u, v) \equiv ac^2(u-b) - u(1-u-v)(1-2u-v) = 0,$$

Steady States of system (I)

$$(0,0), \quad (1,0), \quad (b, 1-b)$$

$(0,0)\ : \lambda_1 = \frac{1}{c}$ and $\lambda_2 = -\frac{ab}{c}$ $\Rightarrow$ saddle point

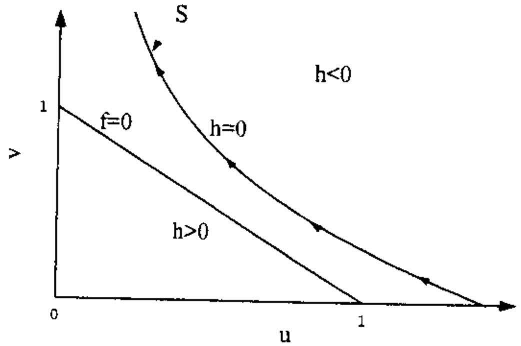
$(1,0)\ : \lambda_1 = -\frac{1}{c}$ and $\lambda_2 = \frac{a(1-b)}{c}$ $\Rightarrow$ saddle point

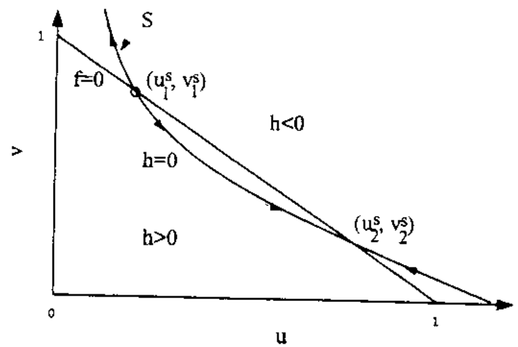
$$\lambda_1, \lambda_2 = \frac{-bc \pm \sqrt{b^2c^2 - 4a(1-b)[c^2 - b(1-b)]}}{2[c^2 - b(1-b)]}$$

$$(b, 1-b)\ : \begin{cases} \text{stable node} & \text{if } c^2 > b(1-b) \text{ and } 0 < a \leq a^\star \\ \text{stable focus} & \text{if } c^2 > b(1-b) \text{ and } a > a^\star \\ \text{saddle point} & \text{if } c^2 < b(1-b) \end{cases}$$

Singularity Curve

$$S = \{(u,v) \in R_+ \times R_+ \mid h(u,v) = c^2 + u(1-u-2v) = 0\}$$





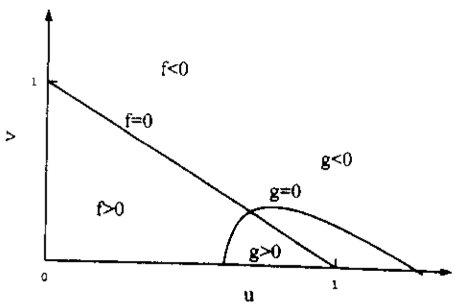
We look for nonnegative solutions of (I) satisfying the boundary conditions

$$(12) \qquad \begin{array}{ll} u(-\infty)=1, & v(-\infty)=0, \\ u(+\infty)=b, & v(+\infty)=1-b \;. \end{array}$$

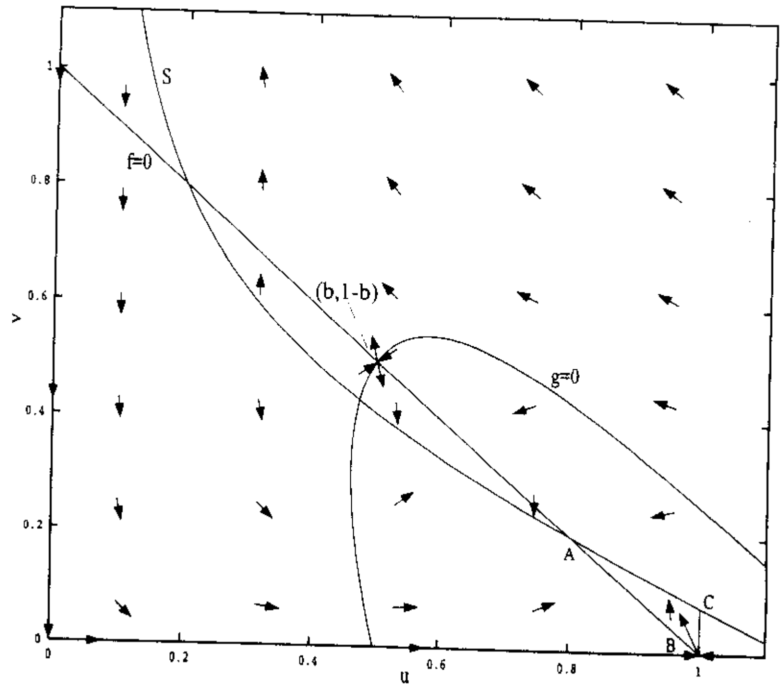
These solutions correspond to orbits in phase plane connecting the steady state $(1,0)$ to $(b, 1-b)$.

Local stable and unstable manifolds of $(1,0)$

stable : u–axis
unstable : $v = -[1+a(1-b)](u-1)$



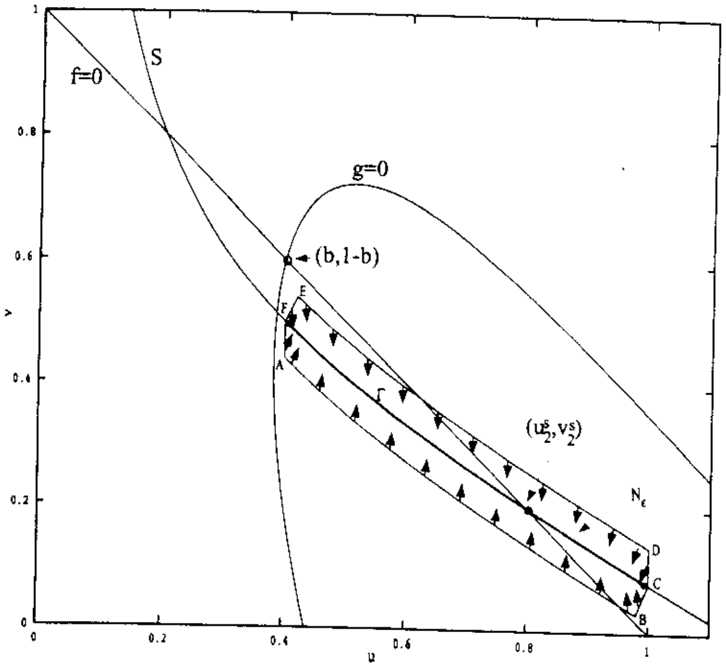
THEOREM 1 *Traveling wave solutions of system (I) which satisfy the boundary conditions (12) do not exist if*
(a) $c < \sqrt{b(1-b)}$,
(b) $\sqrt{b(1-b)} < c < \frac{1}{2}$ *and* $0 < b < \frac{1}{2}$.



$$\Gamma = \{(u,v) \in S \mid g(u,v) > 0,\ b < u < 1,\ 0 < v < 1-b\},$$

$$N_\epsilon = \{Q \equiv (u,v) \mid g(u,v) > 0,\ b < u < 1,\ 0 < v < 1-b, \mathrm{dist}(Q,\Gamma) < \epsilon\}.$$

PROPOSITION 1 *Let $c < \sqrt{b(1-b)}$. For sufficient small ϵ, a solution of (I) having a point z_0 such that $(u(z_0), v(z_0)) \in \partial N_\epsilon \setminus \Gamma$, will have $(u(z), v(z)) \in N_\epsilon$ for all $z > 0$. Furthermore, for some finite z_s $(u(z), v(z)) \in \Gamma$ for all $z > z_s$.*



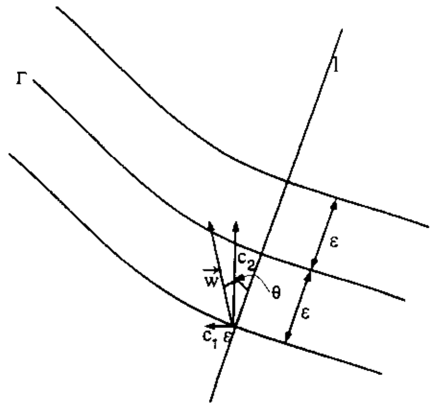
$$u' = \frac{1}{c}u(1-u-v)\ ,$$

$$v' = \frac{v}{c}\ \frac{ac^2(u-b) - u(1-u-v)(1-2u-v)}{c^2 + u(1-u-2v)}\ ,$$

(13) $|u'| \le c_1,\ \ v' \ge \frac{c_2}{\epsilon}$ if $v' > 0$, and $v' \le -\frac{c_2}{\epsilon}$ if $v' < 0$.

Integrating each inequality in (13) from 0 to z we obtain

(14) $$|u(z) - u(0)| \le c_1 z \ \text{ and } \ |v(z) - v(0)| \ge \frac{c_2}{\epsilon}z.$$



THEOREM 2 *Traveling wave solutions of system (I) which satisfy the boundary conditions (??) exist if*
(a) $c > \frac{1}{2}$, *and* $c^2 > 4a(1-b) - 2$,
(b) $\sqrt{b(1-b)} < c < \frac{1}{2}$, $\frac{1}{2} < b < 1$, *and* $c^2 > 4a(1-b) - 2$.
Furthermore, there is a value $a^\star = b^2c^2/4(1-b)[c^2 - b(1-b)]$ *such that if*
(1) $0 < a \leq a^\star$, *the functions* u *and* v *approach* b *and* $1-b$ *monotonically for large* z,
(2) $a > a^\star$, *the functions* u *and* v *approach* b *and* $1-b$ *with an oscillatory behavior.*