Model formalisms, continued; CA, ODE

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Yesterday

- Computational Biology: understanding counter intuitive micro-meso-macro transitions through dynamic modeling
- model requirements: *unique next state function*
  FSM $->$ (multiple) attractors ($+$ Garden of Eden states)
- model formalisms as constraints
  FSM subsystems: CA
  – very simple rules $->$ maximally complex behavior
  – Mesoscale patterns – Zoo

QUESTIONS?

TODAY

- CA as modeling tool: examples
- alternative constraint (shortcut): ordering of states ODE
- CA , ODE as dynamical systems: common/non-common concepts/features.

CA as ....

prototype local interactions give complex behavior

- dynamical system
- experimental mathematics , artificial physics(Ulam)
- artificial life (von Neumann, Langton)
- 'new' physiscs (Wolfram):

  ....Universe is 3D CA *"we only have to find the transition table"*
- **modeling tool** *particle based* (Toffoli)
- (pattern enhancer/classifier (e.g. proteins))
- (NOT bad PDF)

Paradigm system

generic behavior, counter example - existence proof

often used generalizations

- probabilistic next state function
  - (deterministic "noisebox")
  - pseudo random generator: SEED
- asynchronous updating

  Note: synchrony implies global control!

  Timescales

  information transfer vs particle conservation
- probabilistic neighbor - choice (within local NB)

can be approximated with "true" CA

Spread of neutral genes vs Diffusion in CA
global vs local particle conservation

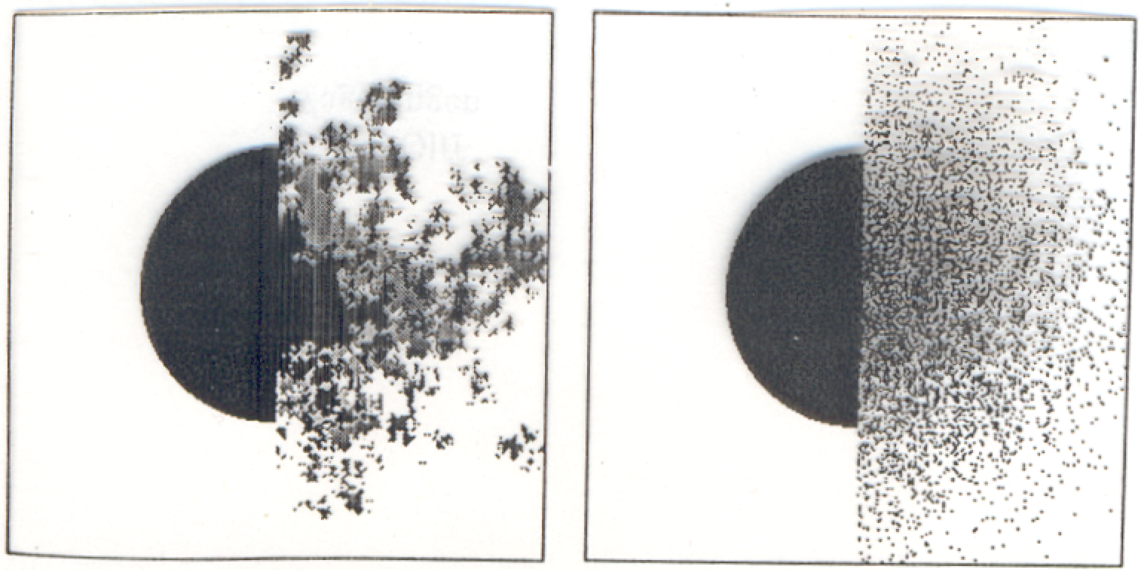


Figure 9.3: (a) Pseudo-diffusion, obtained with a "copy from a random neighbor" rule, vs genuine diffusion (b). Both figures are split-screen, starting from a disk, showing half "before" and half "after."

Margolus Algorithm, Lattice gasses

From Toffoli, Cellular Automata Machines, 1988

Example
CA based models:
not only micro scale and macroscale
MESOscale patterns

Themes:

Setting Baseline expectation

what needs explanation?

Default dynamics vs (evolutionary) selected behavior vs optimal behavior

Lymphnode B-cell nodules

Example: Lymphnodes: B/Tcell nodules

questions: Why this pattern

– *how established*

– *why did the system evolve such that it makes the pattern*

Model

- cross-section
- states: presence/absence of cell B/T at position
- nextstate: birth/death
- influx/outflux of cells (cf particle conservation)
- *Competition for space*

note: clonal selection

The Lymphoid System

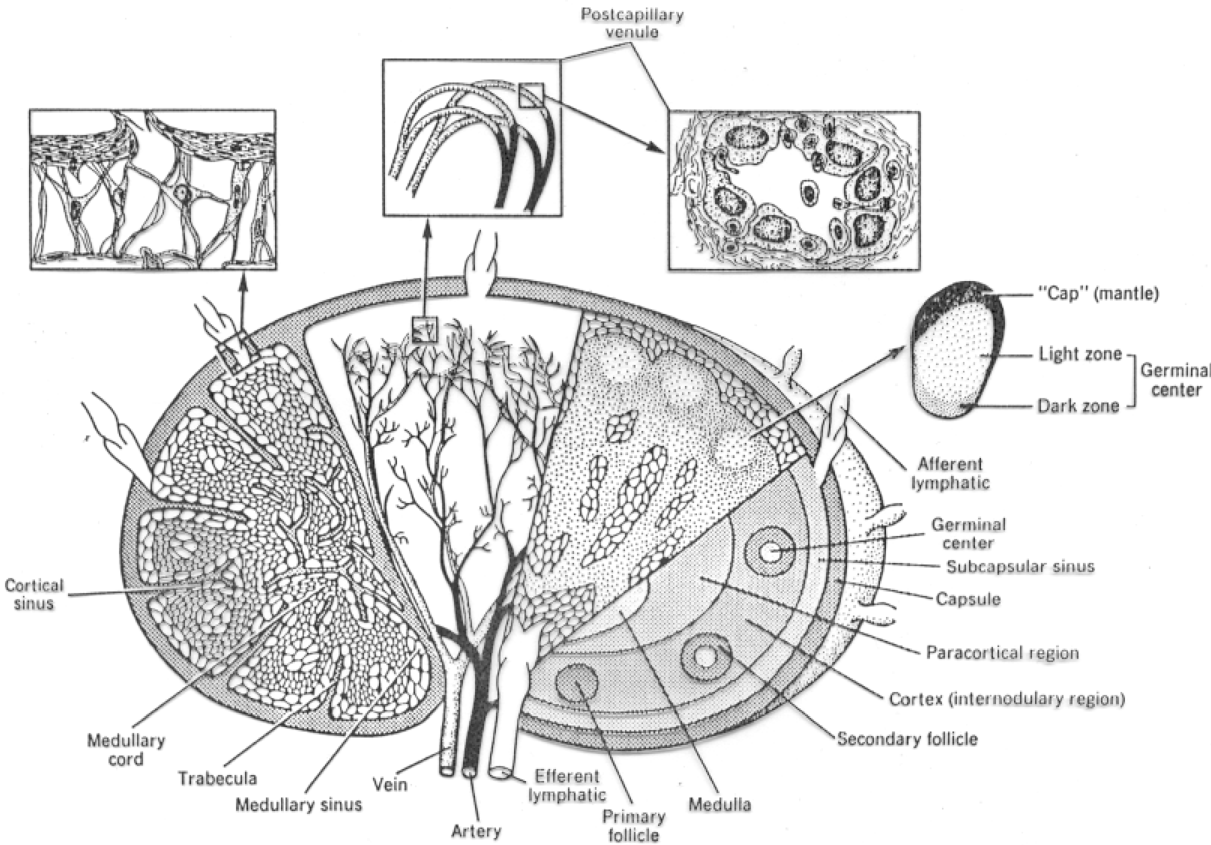


Figure 4.23. Histological organization of a lymph node. The four wedges of the node represent, from left to right, the reticular framework, the circulatory system, the cellular components, and the main structural features in diagram. The four drawings outside the node itself are magnified views of the indicated areas. The third from the left shows the passage of lymphocytes through the postcapillary venule.

The Lymphoid System: CA rules

Next state of empty cell, dependent of number of neighbours of each cell type.

T cells \ B cells	0	1	2	3	4	5	6	7	8
0	.	.	.	.	.	.	.	.	.
1	.	B	B	B	B	B	.	.	
2	T	T	T/B	B	B	B	.		
3	T	T	T	T/B	B	.			
4	T	T	T	T	T				
5	T	T	T	.					
6	.	.	.						
7	.	.							
8	.								

T: T cell; B: B cell; T/B probability, 0.5 for T cell or B cell.

Next state of empty cell, dependent of number of neighbours of each cell type.

T cells \ B cells	0	1	2	3	4	5	6	7	8
0	.	.	.	.	.	.	.	.	.
1	.	T/B	B	B	B	B	.	.	
2	.	T	T/B	B	B	B	.		
3	.	T	T	T/B	B	.			
4	.	T	T	T	T/B				
5	.	T	T	.					
5	.	.	.	.					
7	.	.							
8	.								

T: T cell; B: B cell; T/B probability, 0.5 for T cell or B cell.

T/B Cell Segregation

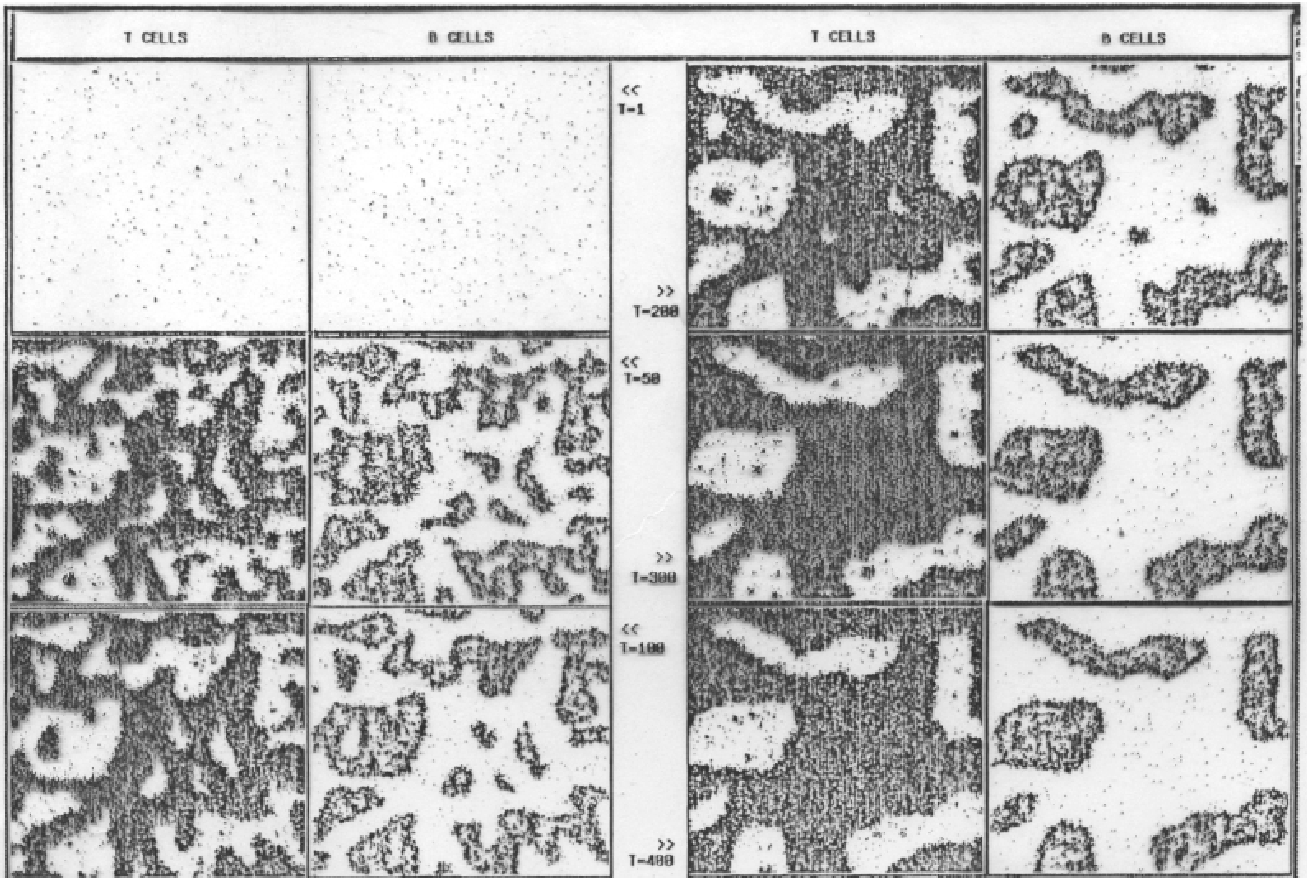


Fig. 2. T/B cell segregation. Large scale patterns develop in cellular automata in which (1) random influx of T cells and B cells occurs (prob 2** −7 each); (2) both cell types proliferate according to the rules given in Table 1 (i.e. both T cells and B cells need T cells to proliferate into an empty space, and they compete for the empty space); (3) diffusion of cells occurs. Time-steps as indicated.

T/B Cell Expansion

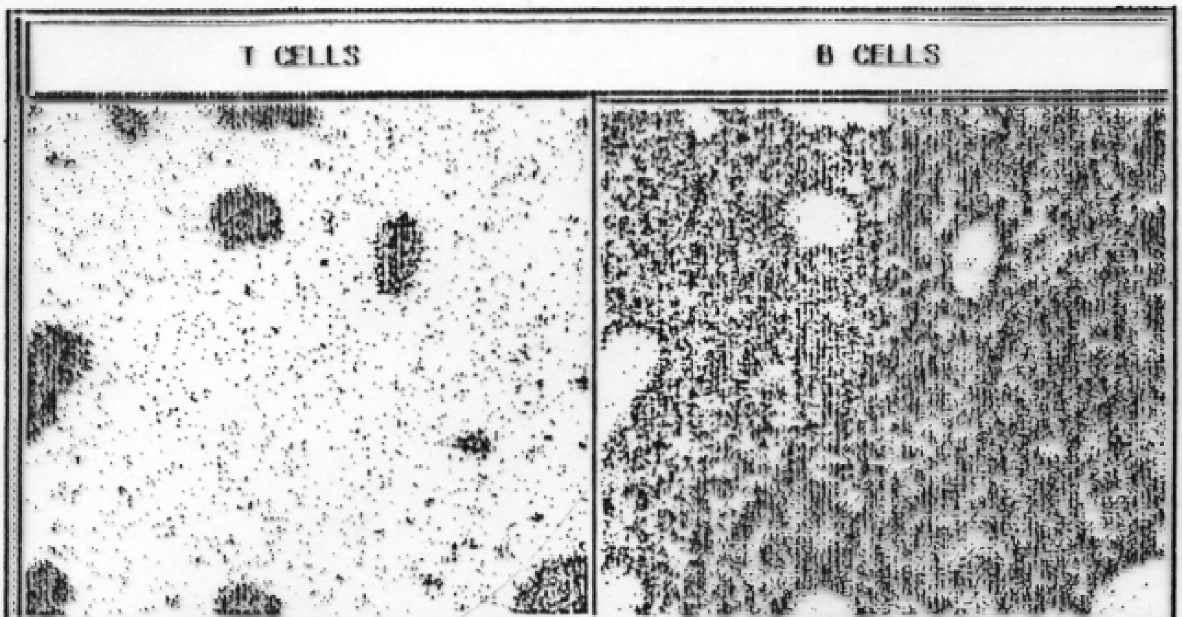
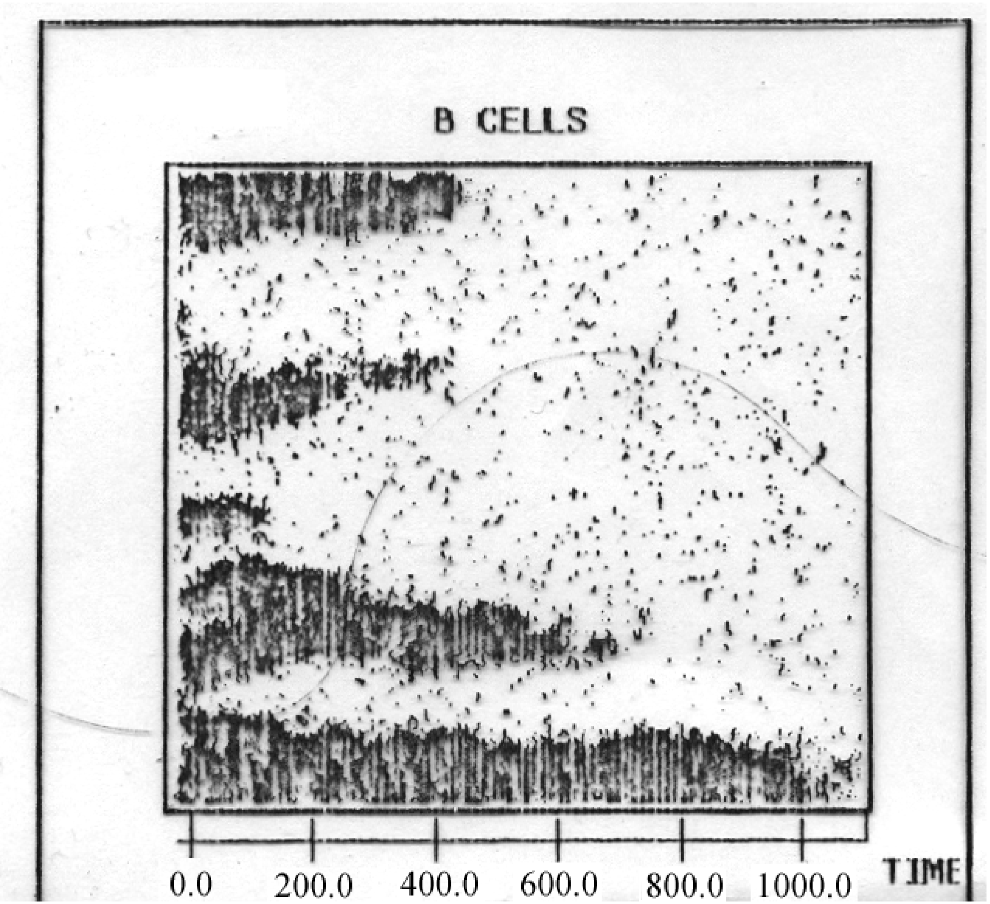


Fig. 3. B cell expansion by increased influx of cells. Identical cellular automaton as in Fig. 2, except that influx of both T and B cells is increased to 2** −6; T = 300.

T/B Cell Expansion



conclusions

Pattern is default (to remain well mixed 'hard')

'Optimal' pattern IS well mixed!

“short cut” on full transition table specification modeling formalisms (heuristics) (continued)

Ordering of states (numerical values of variables)

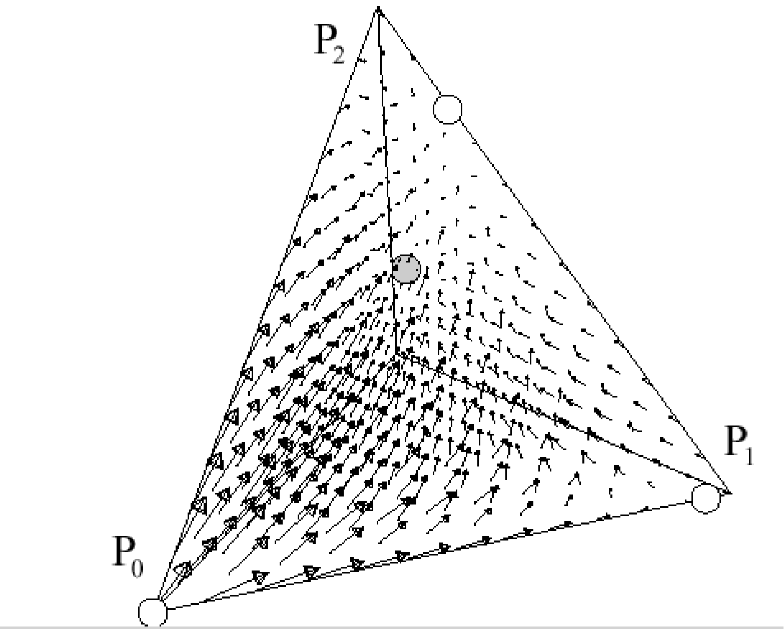
- k Dim state (phase) space (k small)
- transition function (valid for all values)
- *(allows relaxing finiteness)*

MAP: $\mathbf{X_{t+1} = fX_t}$

ODE : $\mathbf{X' = fX}$

Numerical approximation ODE

$$\mathbf{X_{t+\Delta t} = X_t + \Delta t * fX_t}$$



mini Primer (reminder) ODE/MAPS
cf math primer modeling primer GRIND tutorial

Equillibria and Jacobian matrix

State space analysis:
null clines. trajectories, vector fields attractors, bifurcation diagram

fixed points, limitcycles, bi(multi)stability

(deterministic) chaos

Studying (nonlinear) ODE (2D): equilibrium points

Stable equilibria

1. Stable node $\lambda_1 < 0; \lambda_2 < 0$ real
2. Stable spiral $\lambda_{1,2} = \alpha \pm i\beta; \alpha < 0$

Non-stable equilibria

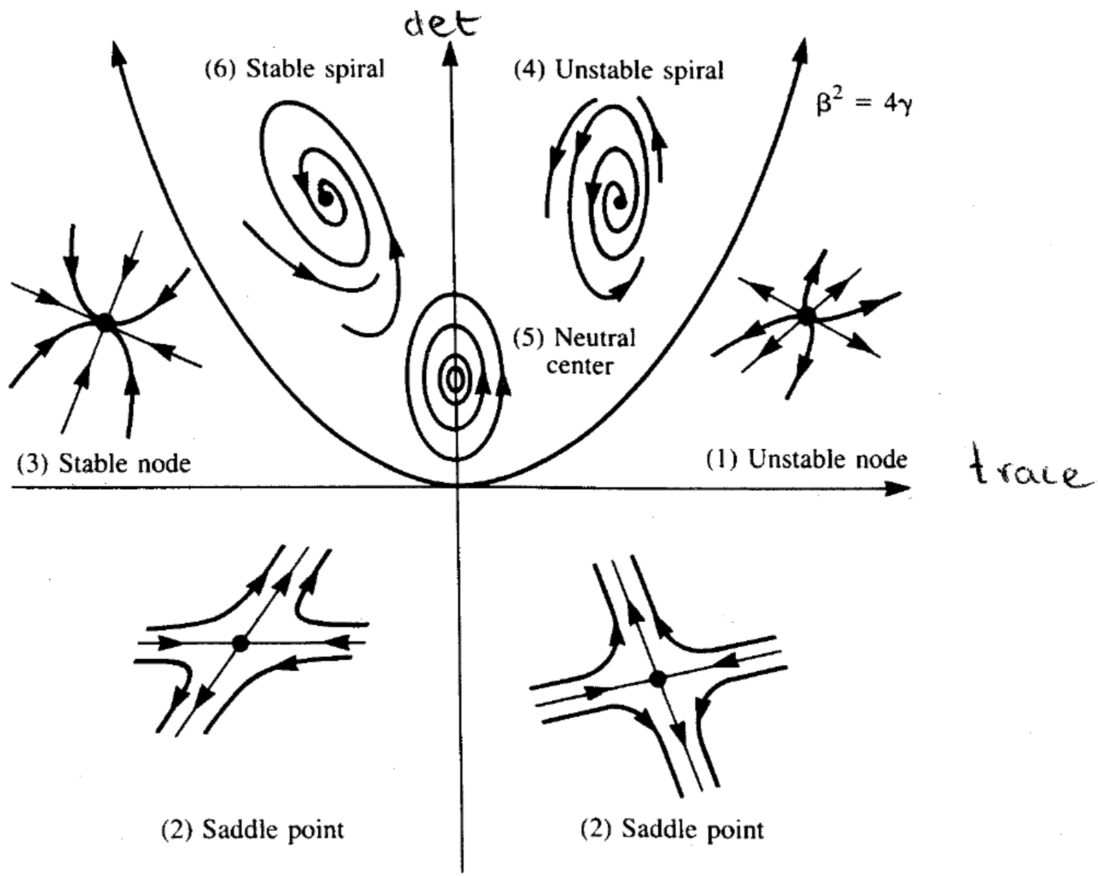
1. Non-stable node $\lambda_1 > 0; \lambda_2 > 0$ real
2. Non-stable spiral $\lambda_{1,2} = \alpha \pm i\beta; \alpha > 0$
3. Saddle point $\lambda_1 < 0; \lambda_2 > 0$; or $\lambda_1 > 0; \lambda_2 < 0$ real

$\lambda_{1,2}$: eigenvalues of Jacobian matrix
Jacobian matrix: partial derivatives at equilibrium

Definition 8 *The trace of the matrix* $\begin{pmatrix} a & b \\ c & d \end{pmatrix}$ *is* $trA = a + d$.

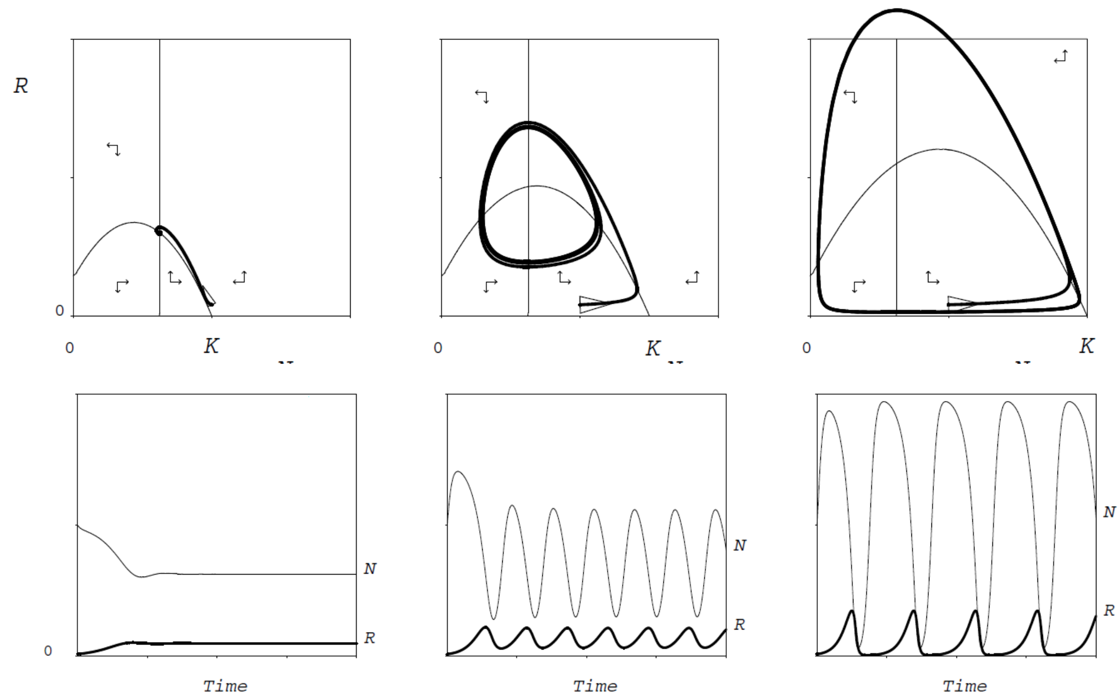
The determinant of the matrix A is $detA = ad - cb$

$$\lambda_{1,2} = \frac{trA \pm \sqrt{D}}{2} \quad where \quad D = (trA)^2 - 4detA$$



Studying (nonlinear) ODE (2D): phase-plane analysis (== state space analysis)

Nullclines: set of states for which derivative is zero
Trajectory: set of states visited from initial condition to time=t
Vector field: direction of change at selected states
Attractors: set of states visited - after "enough time"
fixed points; limit cycles
Bifurcation diagram: attractors as function of parameter



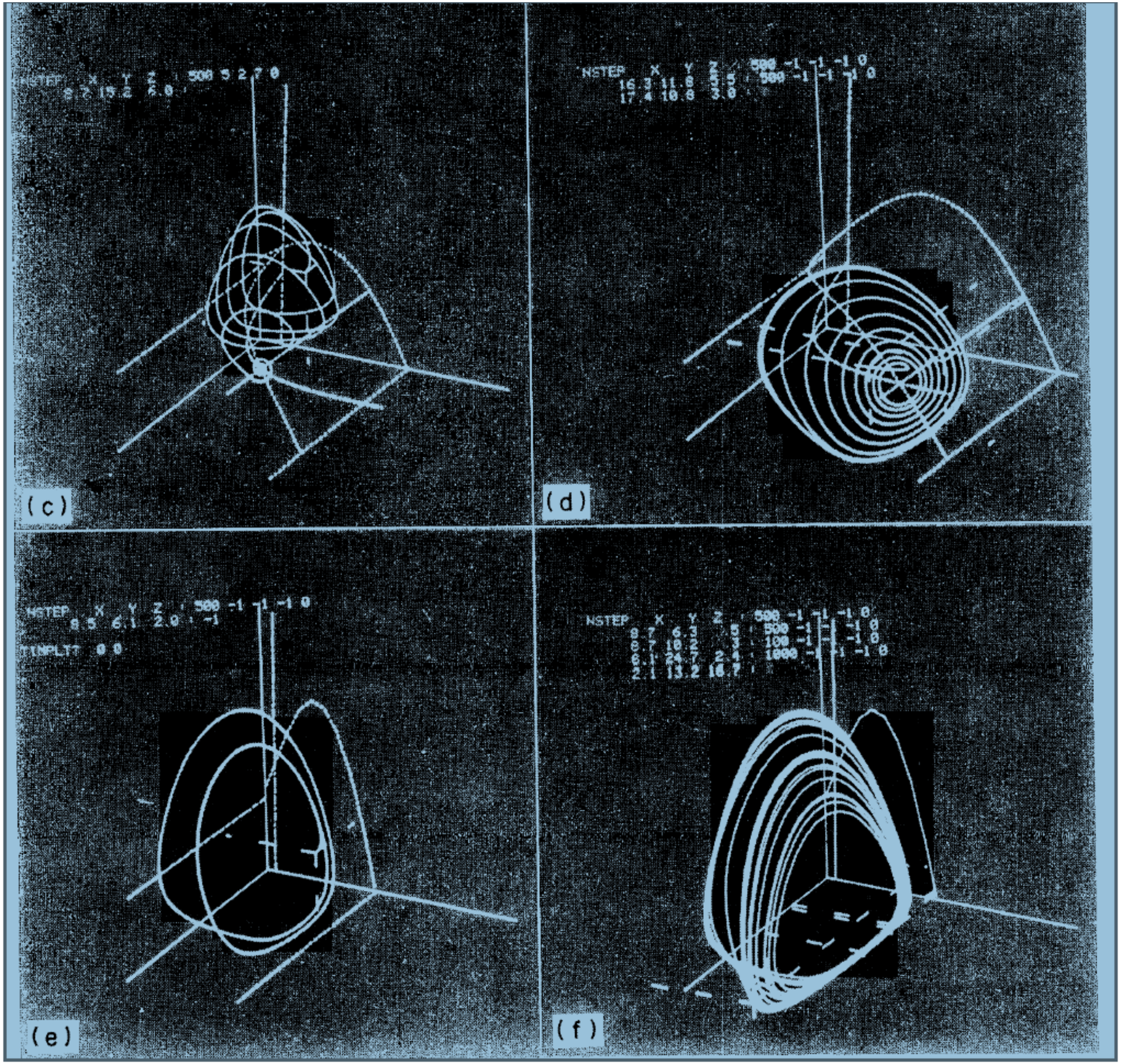
3D

new type of **attractor**:

Deterministic Chaos

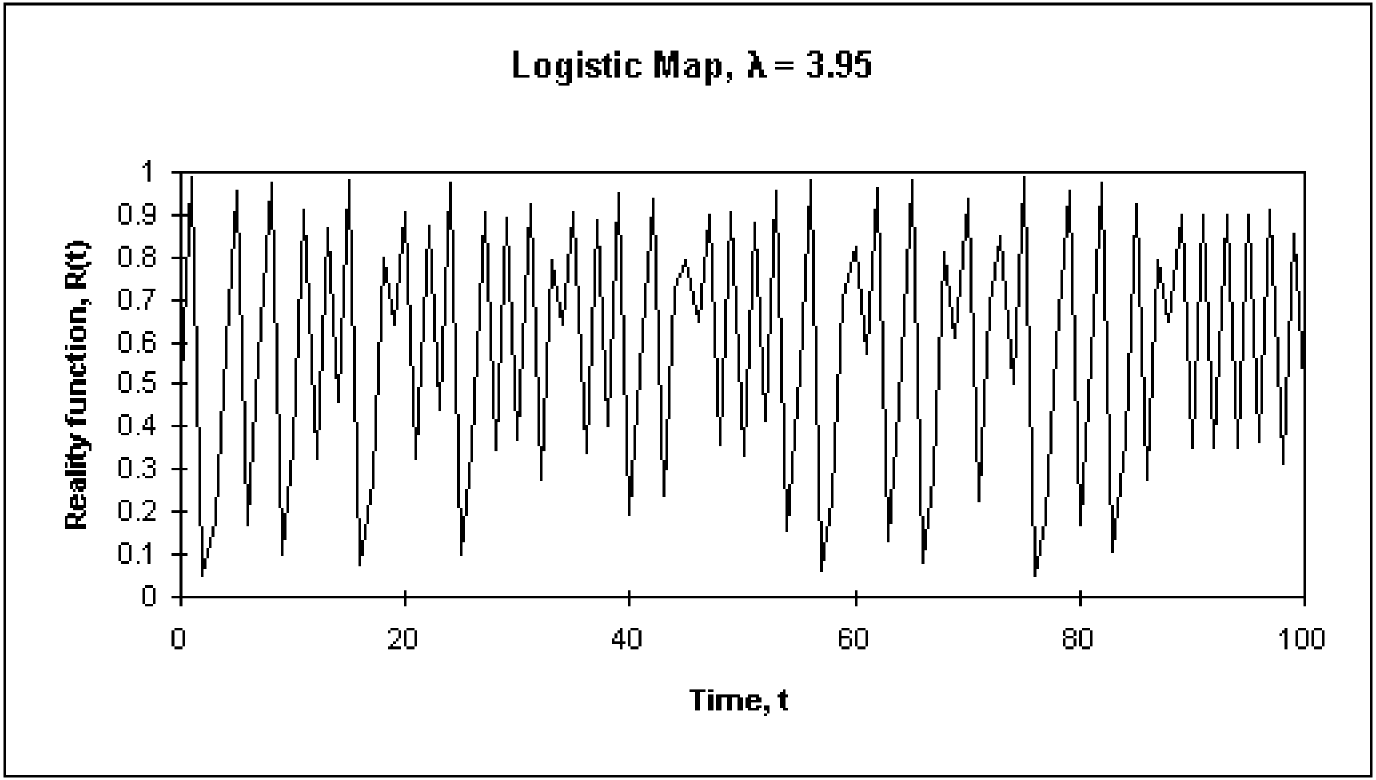
Non-periodic

(period doublin



MAPS: also deterministic chaos in 1D maps

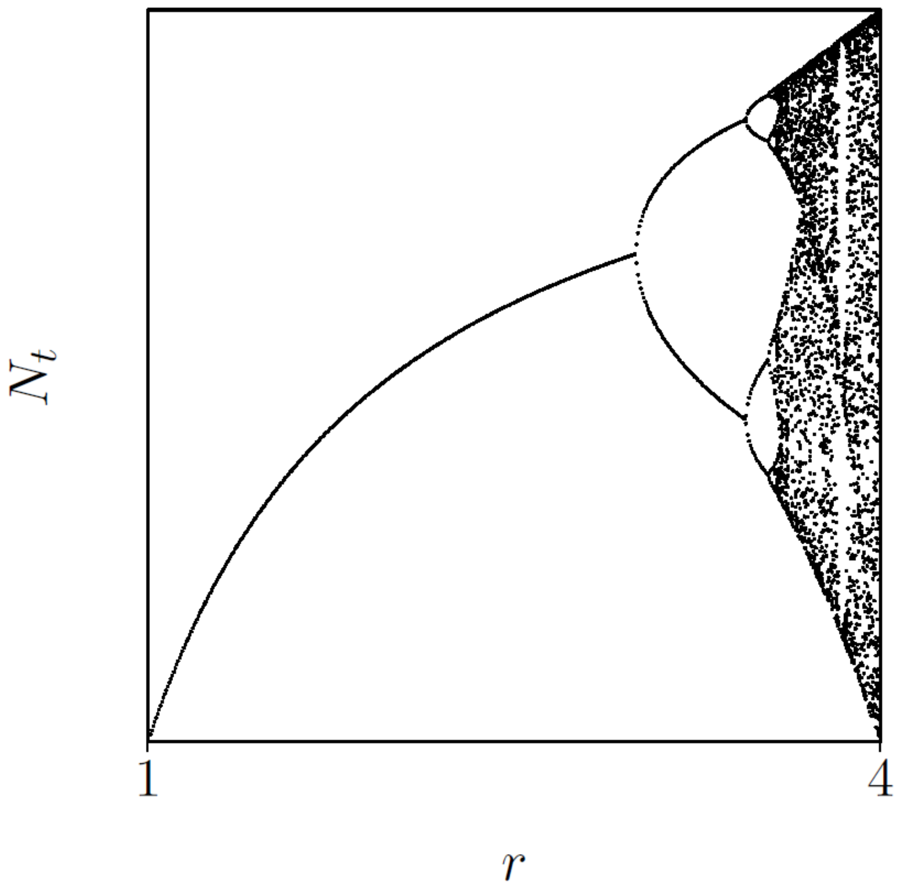
best known example: logistic map $N_{t+1} = \lambda N_t(1 - N_t)$

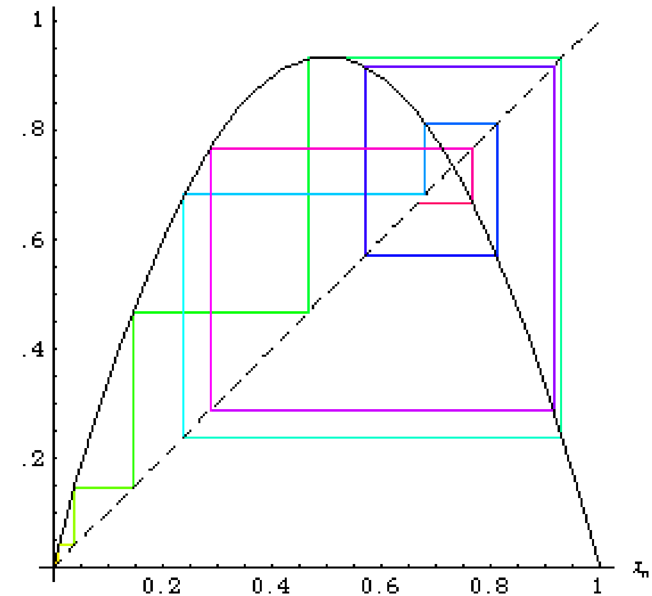


MAPS: also deterministic chaos in 1D maps

best known example: logistic map $N_{t+1} = rN_t(1 - N_t)$

bifurcation diagram, Takens plot, cobweb





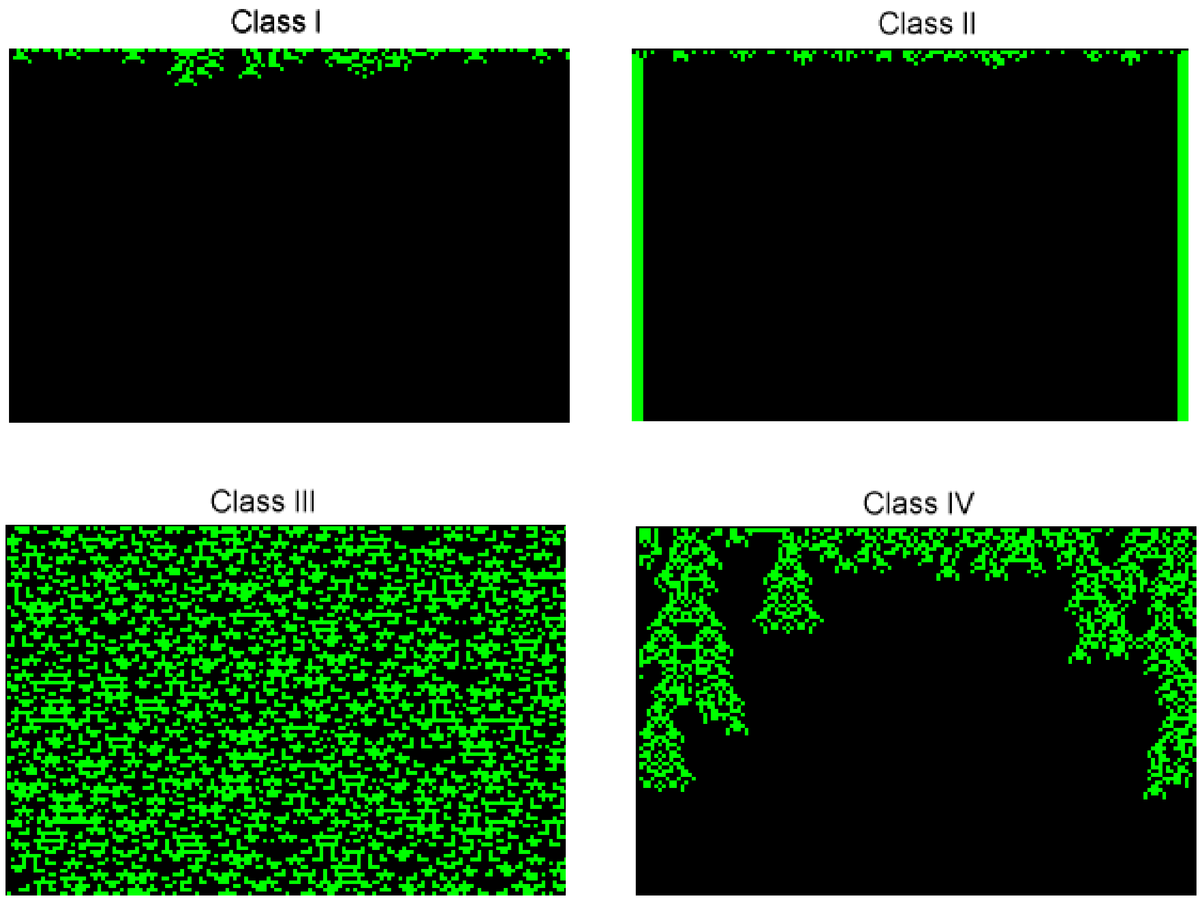
(autonomous) Dynamical systems: basic properties

- unique nextstate function (cf vector field)
- attractors: fixed point, limit cycle, chaotic attractor
- basin of attraction
- transient

manifestation in CA

CA classification (Wolfram)

eyeball spacetimeplots of (1D) CA's , random initial conditions



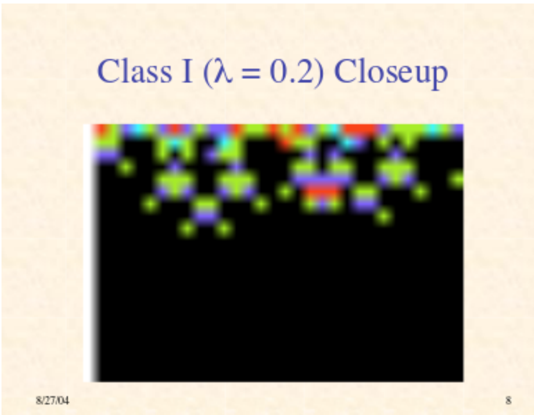
High dimensional chaos

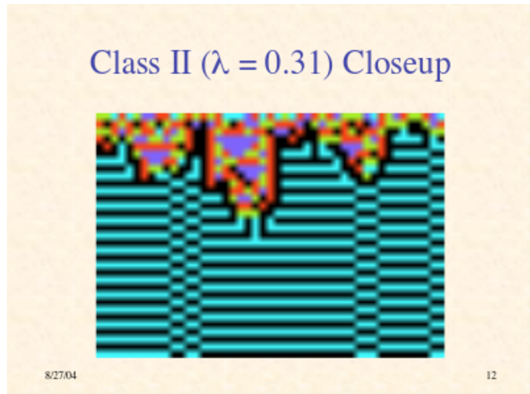
Universal computation

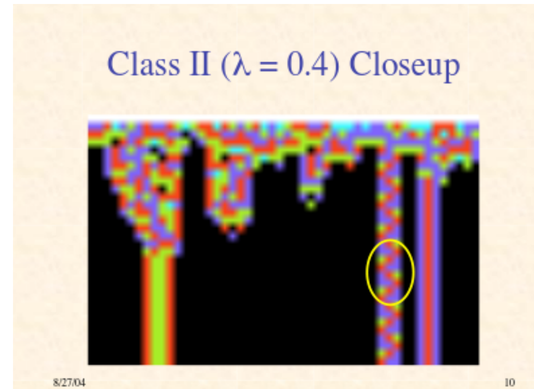
~ random

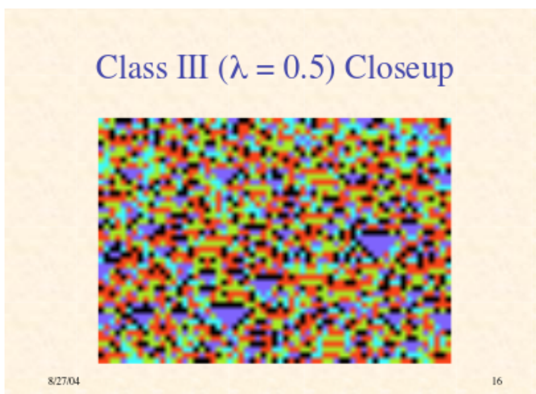
# of 1 ~ constant

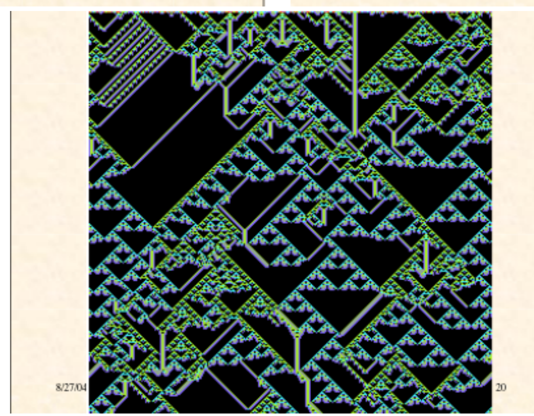
more eyeballing











Classification of CA's (Wolfram, Langton)

Switch to random initial conditions (1D - Elementary CA's)

	spatial pattern	non-spatial analogue
Class I :	to uniform state	fixed point
Class II a	domains, localized	limit cycles
Class II b	idem non-stationary	idem
III	non(>>)-periodic , non-localized	chaos (high dim.)
Class IV	loc. + non-loc., long transient	universal computation

Order parameter λ = Fraction of rules to the non-quiescent state(s)

I——IIa ——IIb-IV-III——

IV "vanishing small" - important???

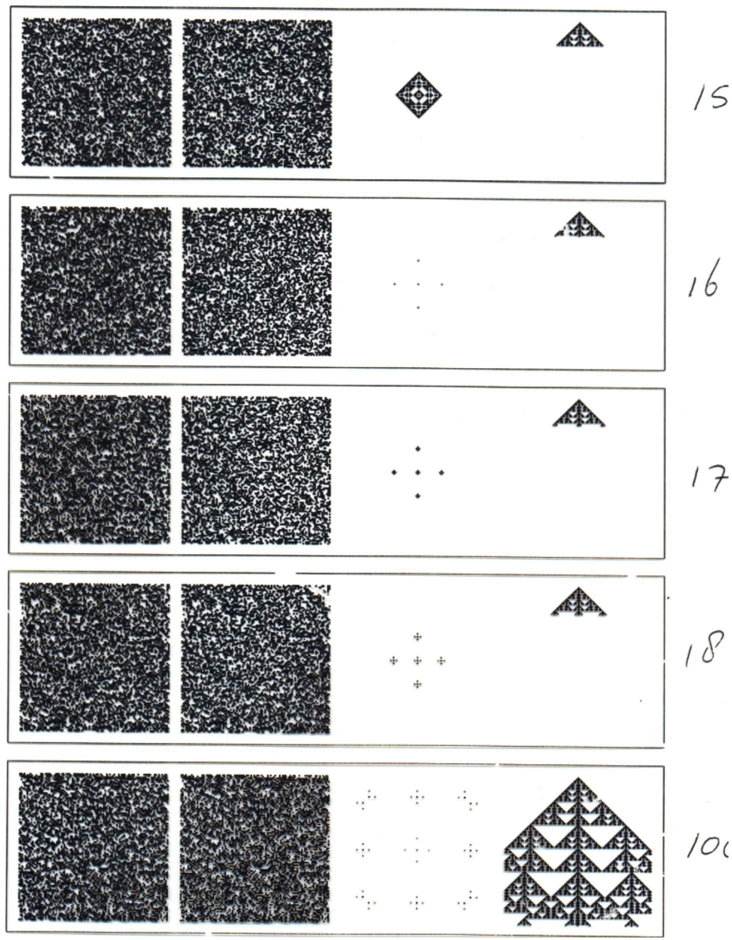
viz Modulo Prime, Game of Life, Voting

Almost all cases

high dimensinal chaos and random noise

Modulo Prime: ($\lambda = .5$) type 3 chaos

random IC, one bitflip difference



Comparing/combining modeling approaches
Model entities, model observables, modeltransformations (1)

CA and/or ODE

Example: Modeling birth/death processes
Dynamical system: fixed set of states/variables,interactions

How to model a variable set of individuals?

- In CA (discrete space/time):
  fixed set of automata (patches)
  individuals as state of patch of space.
  birth: s=0 (empty square) copies state of a nb
  death: s=1 (occupied by idividual) $->$ s=0 (with prob d)
  'population' as observable.

- in ODE (continuous time/variables): (e.g. $dN/dt = aN - bN^2$)
  MAPS (discrete time, cont variables): (e.g. $N_{t+1} = (a+1)N_t - bN_t^2$)

  fixed set of variables (here 1)
  birth/death changes in values of variables.
  'population' is model entity AND observable.

relating CA en ODE models: ODE as MEAN FIELD 'APPROXIMATION' of CA

$$dN/dt = aNE/T - dN$$

$$dN/dt = aN(1 - N) - dN$$

$$dN/dt = (a - d)N - aN^2$$

E is empty space

-'simplification' to population based description
- mixing (localness vs pattern formation)
- NOTE: lumping/naming of parameters.

VS Mean Field Assumption(!)