EXACT FORMULATION OF ISING MODEL TRANSITIONS BETWEEN SIX MAGNETIC PHASES

by

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INFORMS 2018 Session Chair

ITS SUMMIT 2019 Presentation

NECSI ICCS 2020 Presentation

Model: ADama Cellular Automaton[1]

Built upon: PyCX 0.3 Realtime Visualization Template

PyCX 0.3 Realtime Visualization Template: Written by Chun Wong

Revised by Hiroki Sayama

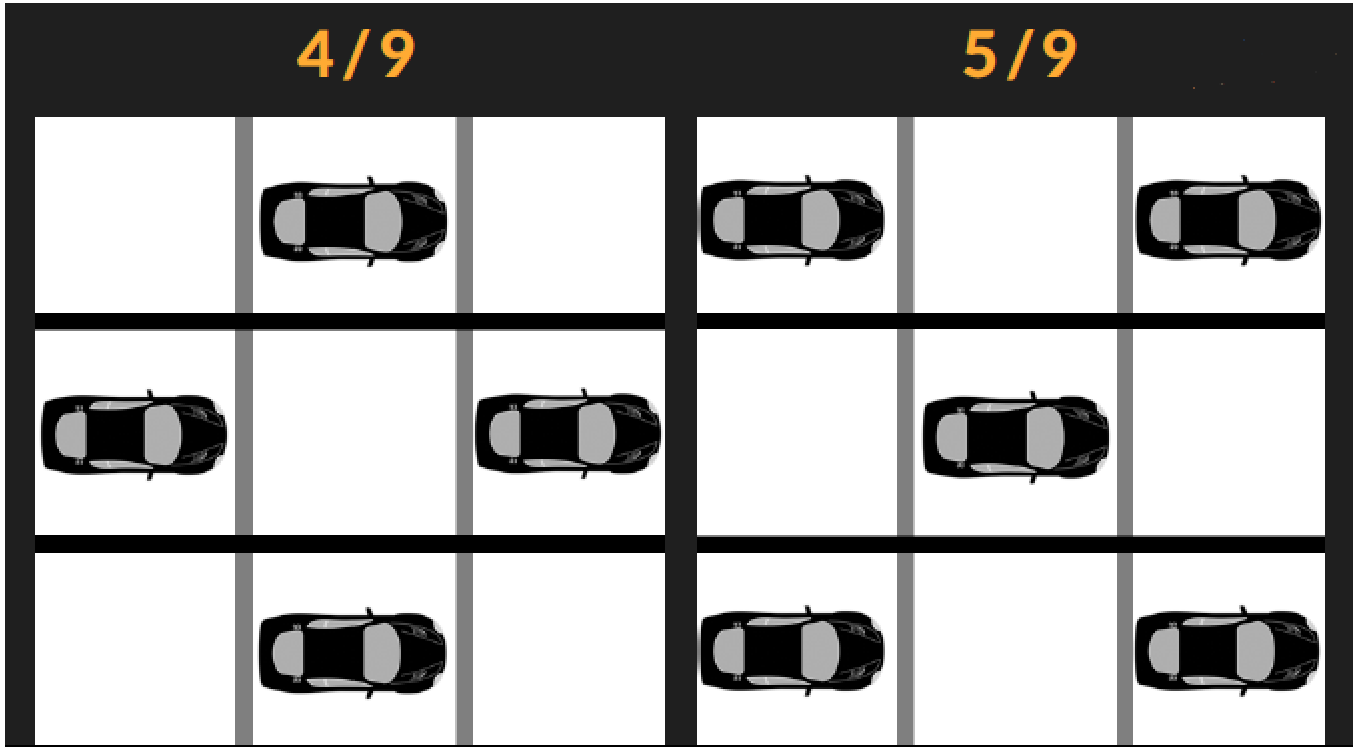
Requires PyCX simulator to run

PyCX available from: https://sourceforge.net/projects/pycx/

1. https://github.com/goktu/ADama/blob/master/cellularautomata.py

Model: ADama Checkerboard

Hypothetical optimal car formation in a 3x3 grid – «zipper merge»



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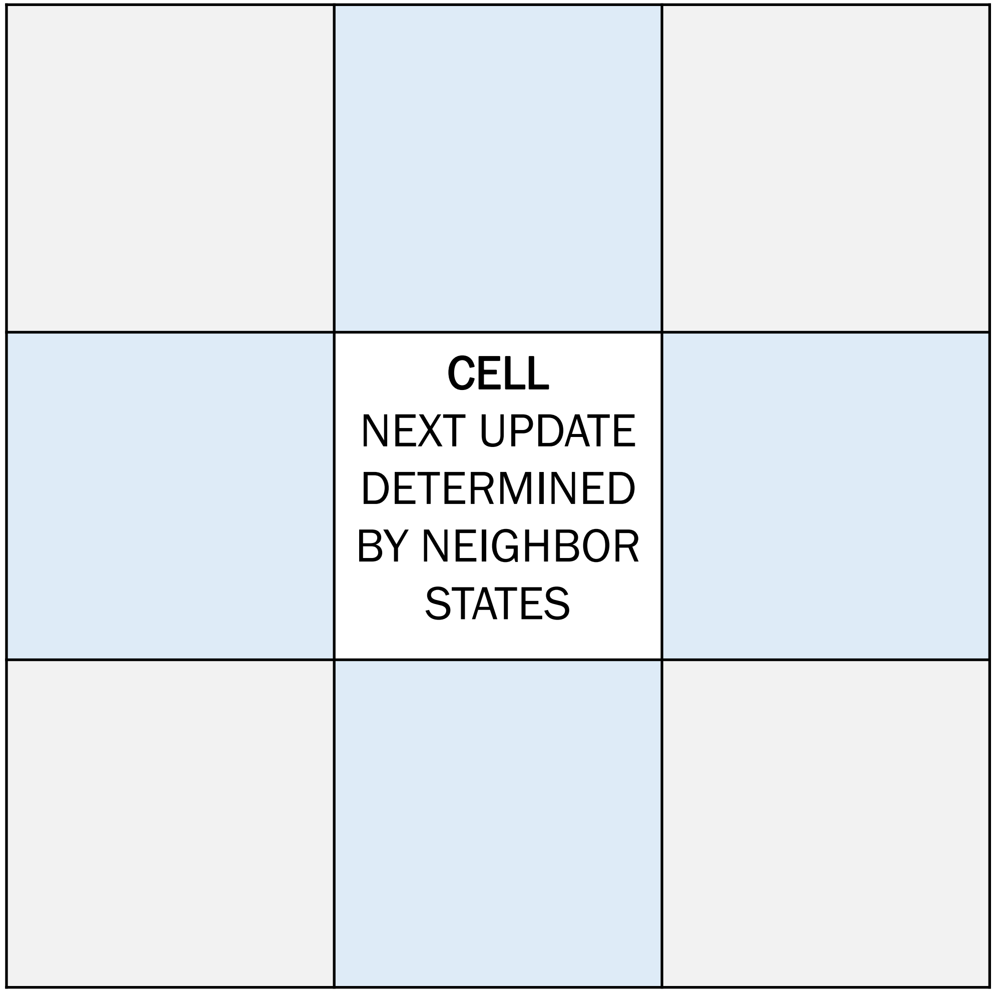
https://www.abstractsonline.com/pp8/#!/4701/session/2099
https://www.abstractsonline.com/pp8/#!/4701/presentation/19295

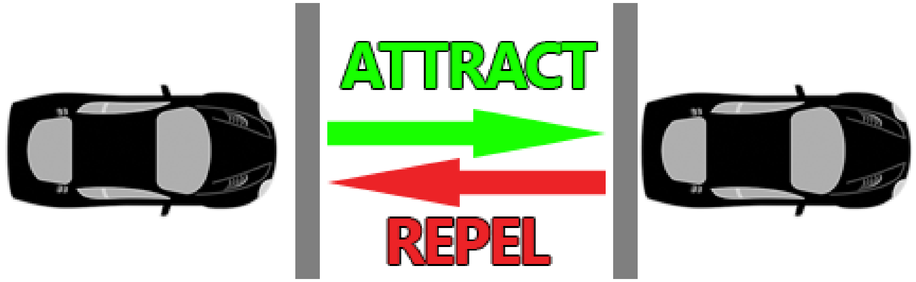
Conventional Cellular Automaton Update

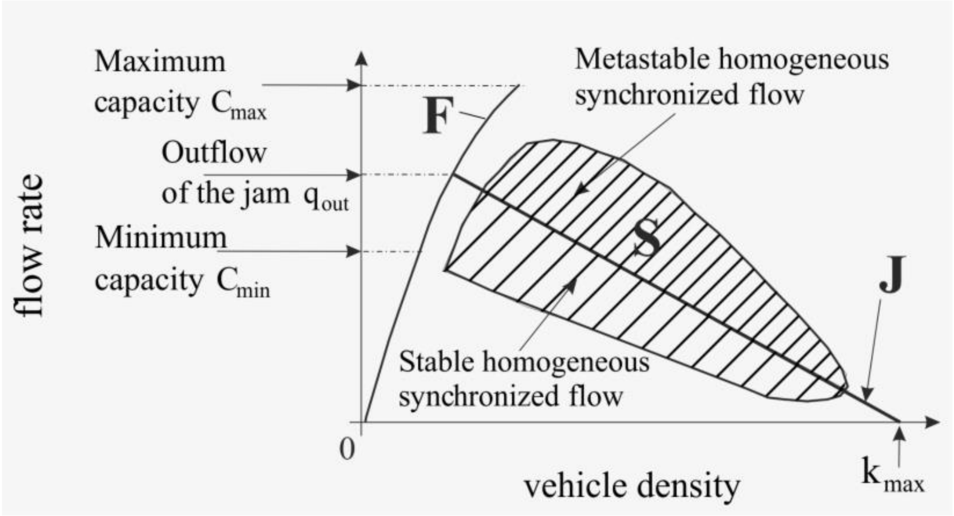


A cellular automaton is a search function around a cell. The update rule is based on the neighborhood.

A well known attractive-repulsive force function is the Lennard-Jones potential. We will explore if uniaxial attractive-repulsive forces can be simulated with cellular automata.

Why Uniaxial Attraction-Repulsion?



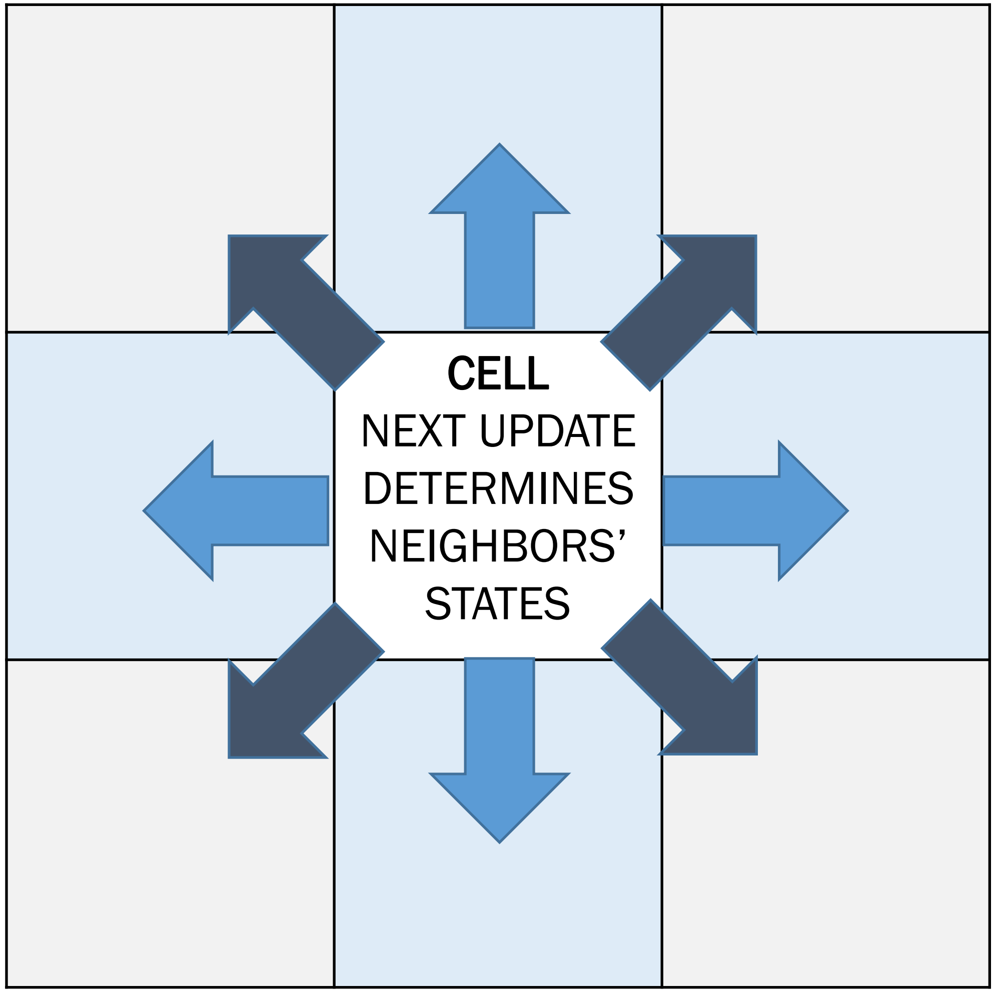


A tailing car is attracted to a frontal car's position, but is forced to leave a trailing distance, a repulsion.

We suggest that this attraction-repulsion is a dipole in the driving direction, and in the normal direction, there is a non-dipole attraction between the vehicles which manifests as lane merging.

Left Below: Synchronized Traffic Flow-Density Graph (Boris Kerner)

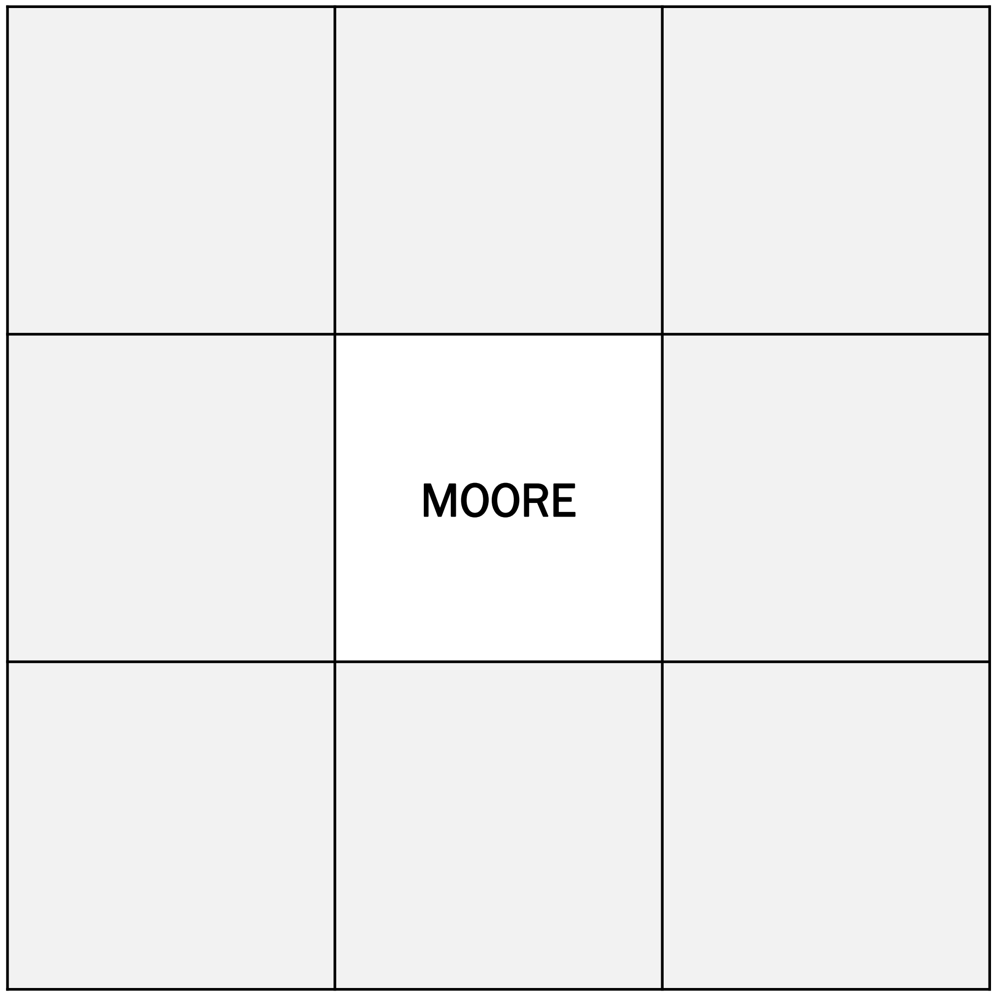
1st Rule: Inverse Cell Update

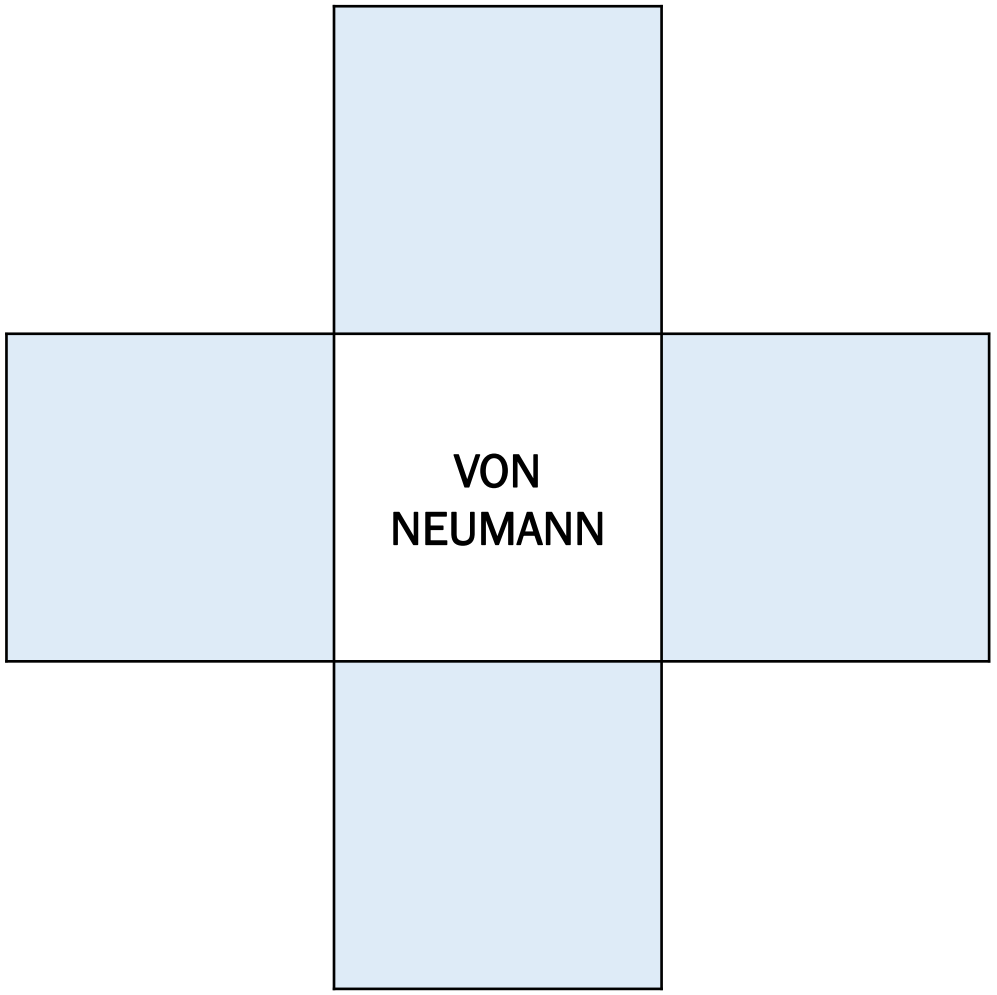


To achieve driving dipole, we have reversed the update of a cell. Cell's state dictates its neighborhood.

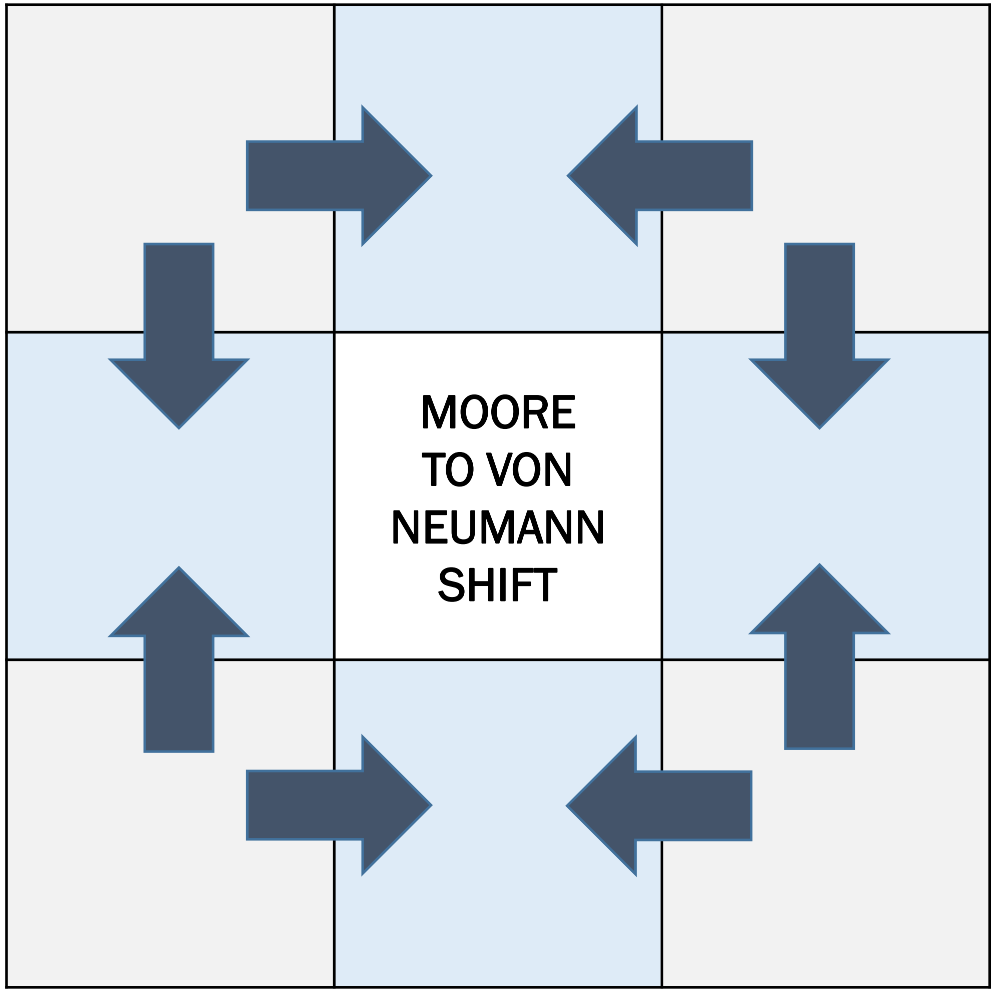
```
elif c[x, y] == 1:
    array1.append(c[x, y])
    for z in range(-1, 2):
        # block generation from randomly distributed points

        #neighbor updating from cell(x,y)
        m = number_of_upper_neighbors(x, y)
        if m == 1:
            nc[x, (y + 1) % L] = 1
```

Moore vs Von Neumann Neighborhoods





2nd Rule: Moore to Von Neumann Shift



This shift is required to simulate renormalization by decimation. We will verify this hypothesis later on.

```
#neighbor updating from cell(x,y)
m = number_of_upper_neighbors(x, y)
if m == 1:
    nc[x, (y + 1) % L] = 1

n = number_of_lower_neighbors(x, y)
if n == 1:
    nc[x, (y - 1) % L] = 1
```

```
k = number_of_right_neighbors(x, y)
if k == 0 and (m <= 1 or n <= 1):
    nc[(x + 1) % L, (y + z) % L] = 1

l = number_of_left_neighbors(x, y)
if l == 1 and (m > 1 or n > 1):
    nc[(x - 1) % L, (y + z) % L] = 0
```

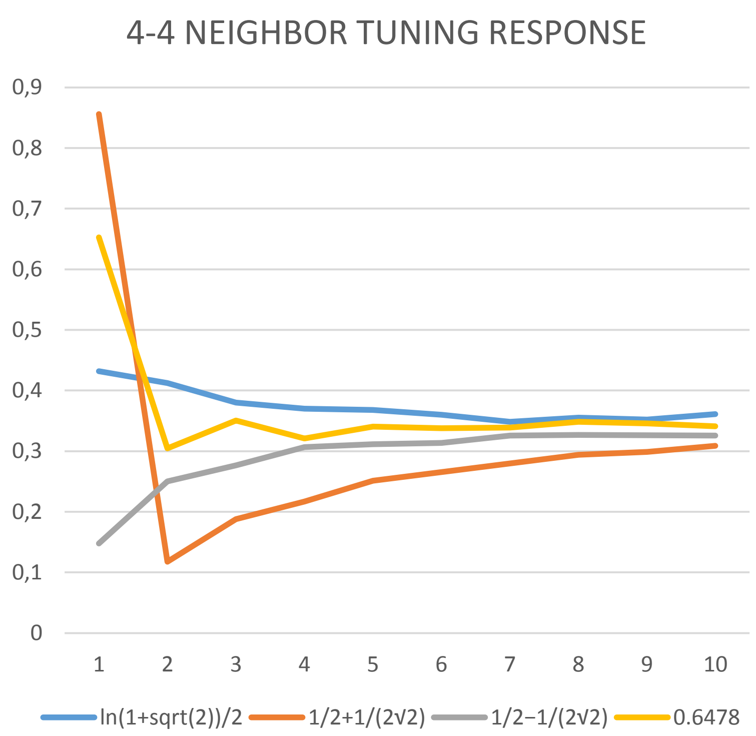
3rd Rule: Neighborhood Configuration

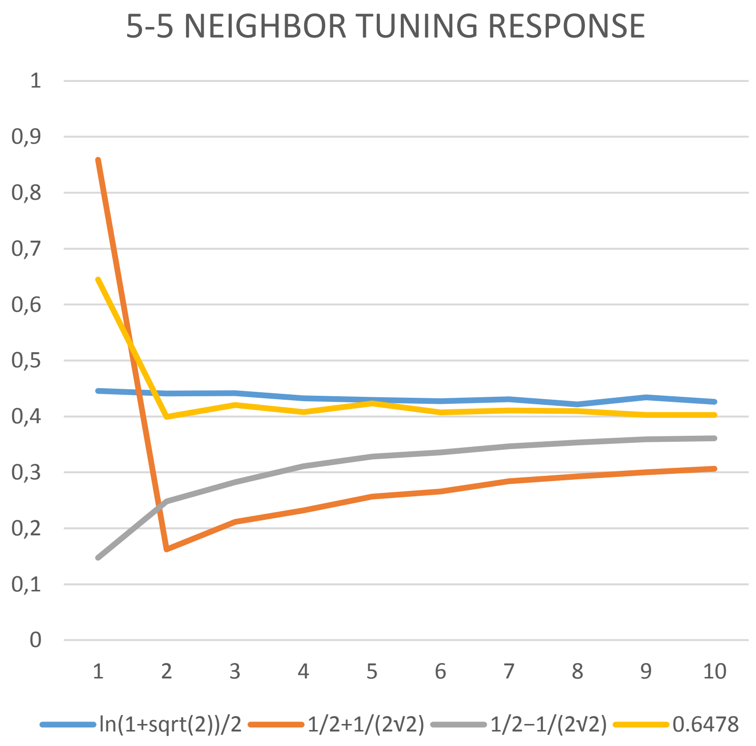
1	1	1
0	TUNING THE NUMBER OF NEIGHBORS WITH STATE 1	0
1	1	1

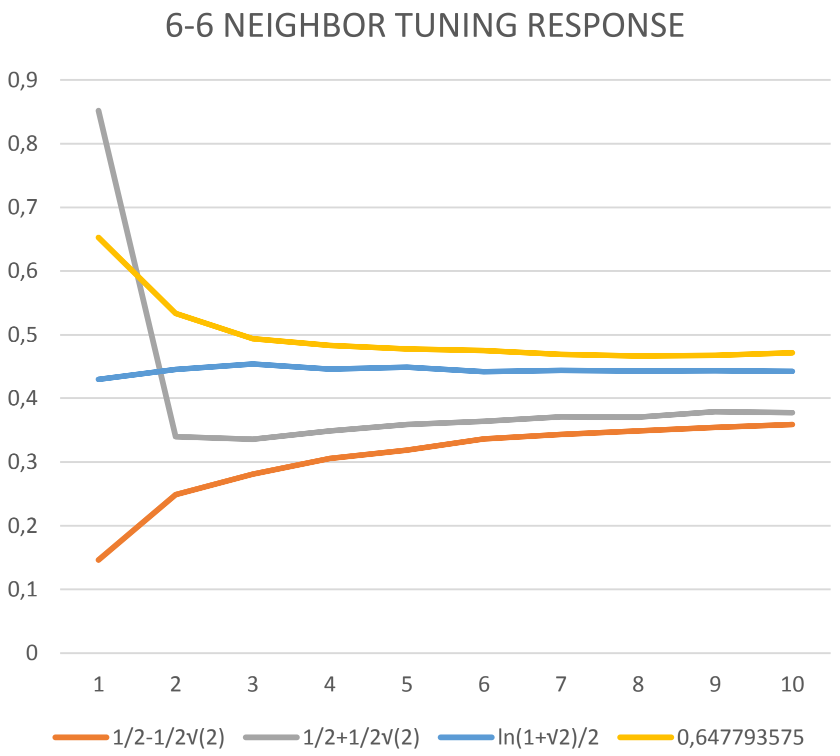
Based on cell's value, neighborhood states are tuned within range. Ideal neigborhood will turn out to be 6.

```
g = number_of_Moore_neighbors(x, y) #CA tuning
if c[x, y] == 0:
    nc[x, y] = 0 if g <= 6 else 1
    array0.append(c[x, y])

h = number_of_Neumann_neighbors(x, y) #CA tuning
if h >= 1:
    nc[x, y] = 1 if g <= 6 else 0
```

Neighbor Tuning for Ising Criticality







Tuning for **4** and **5** neighbors has **Inverse Ising critical temperature** as the highest state **1** cell count.

For **6** neighbors however, there is another maximum susceptibility, corresponding to ferromagnetism.

4th Rule: Coupled Cellular Automata

$$\rho(t+1) = (1-p)\varphi\big(\rho(t)\big)$$

p(1-p): Logistic map

1/8: Moore Neighborhood Average

$$p(1-p) = \frac{1}{8}$$

$$p^2 - p + \frac{1}{8} = 0$$

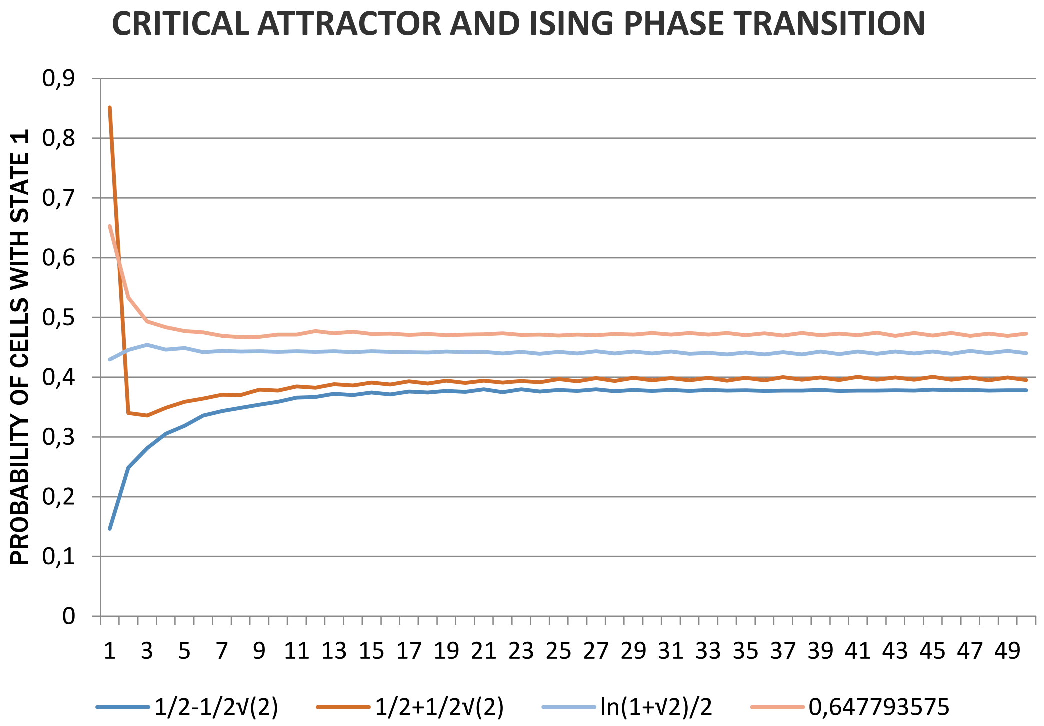
$$p = \frac{1}{2} \pm \frac{1}{2\sqrt{2}}$$

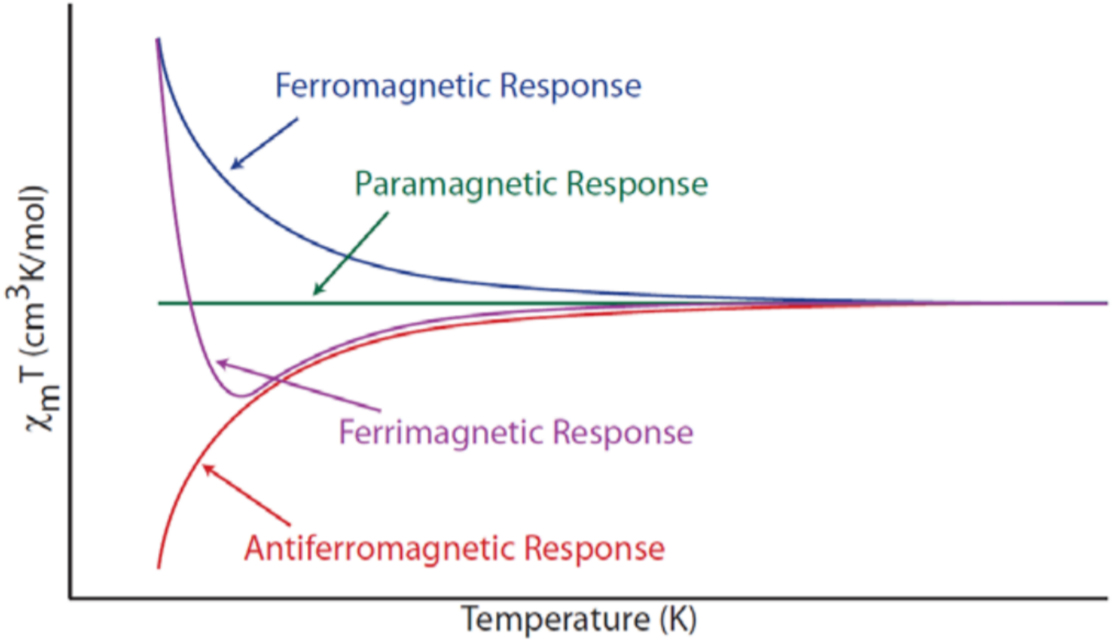
Left Top: Stochastic coupling mechanism evolution equation.[2]

```
if g / 8 > (1 - p) * p:  # coupling function
    nc[(x + 1) % L, y] = 1
elif g / 8 < (1 - p) * p:
    nc[(x - 1) % L, y] = 1
else:
    nc[x, y] = 1
```

2. Synchronization of stochastically coupled cellular automata. Luis G. Morelli and Damian H. Zanette. Phys. Rev. E 58, R8(R) – Published 1 July 1988

Coupling Function – Magnetizing Automaton





2D Ising square lattice model's critical inverse temperature is the **paramagnetic response.**

Upper coupling is slightly striped, which is weak ferromagnetism (**ferrimagnetism**).

Lower coupling is vortex shaped, which is **antiferromagnetic** behavior.

Right Figure: http://bh.knu.ac.kr/~leehi/index.files/MPMS_HIL.pdf

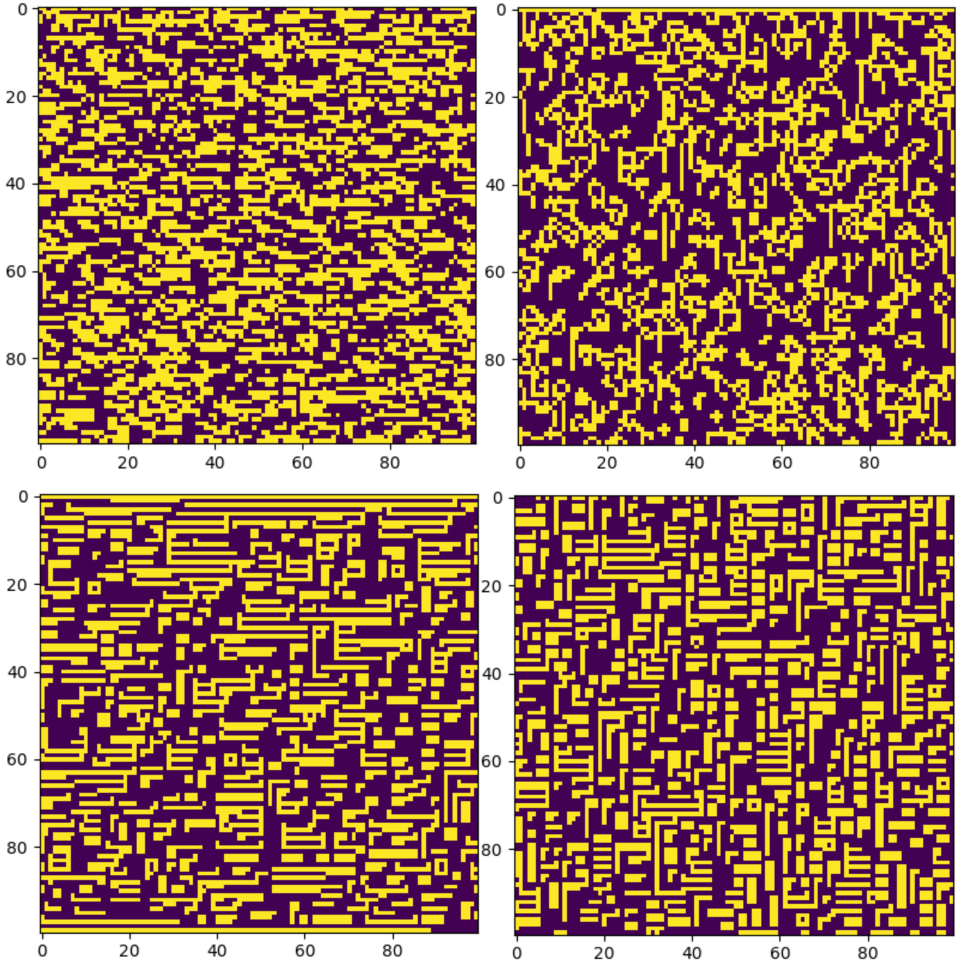
Evolution of Coupled CAs

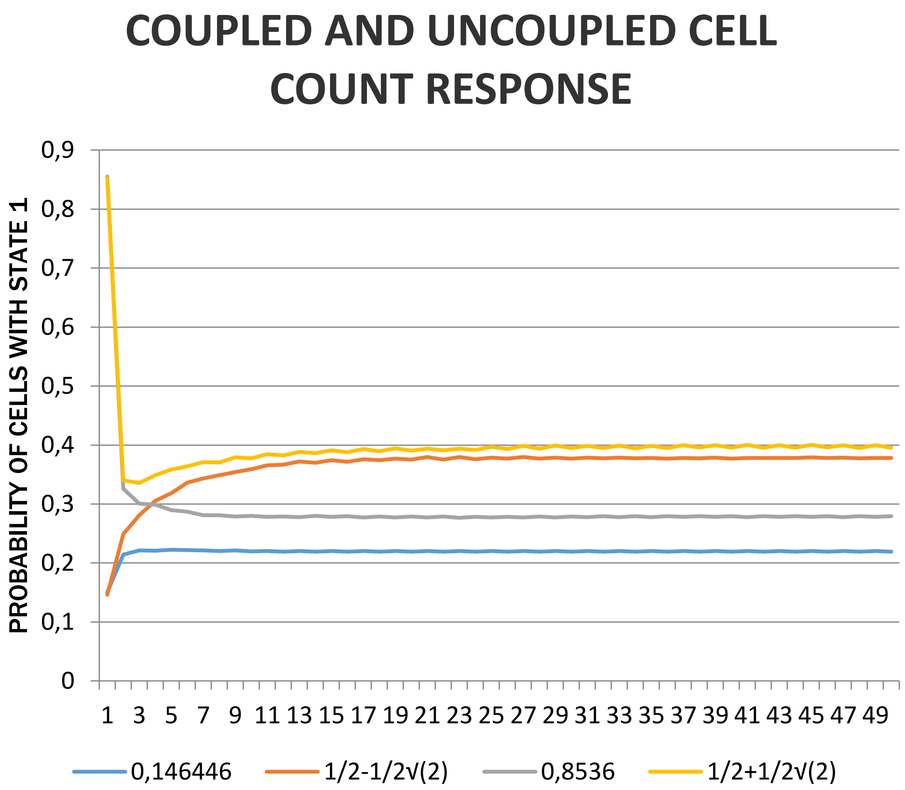
p(1-p): Logistic map; 1/8: Moore average

$$p(1-p) = \frac{1}{8}$$

$$p^2 - p + \frac{1}{8} = 0$$

$$p = \frac{1}{2} \pm \frac{1}{2\sqrt{2}}$$

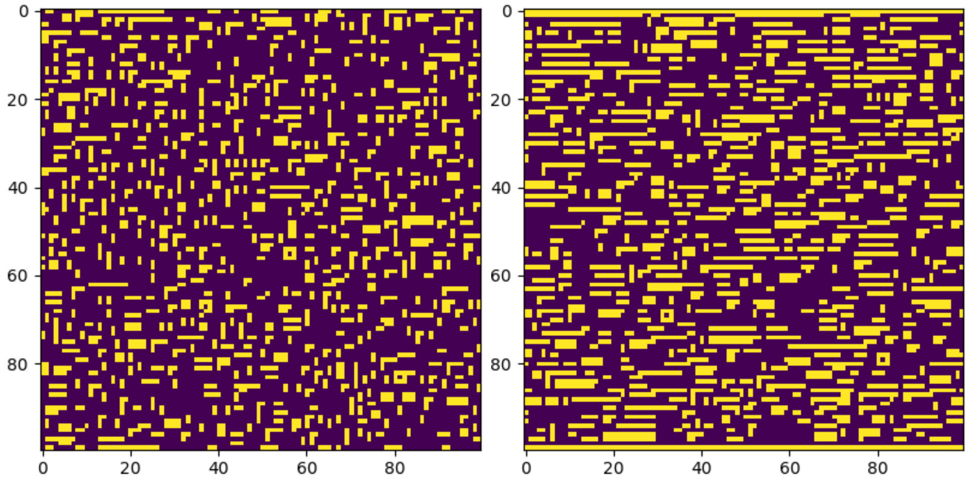




CLOCKWISE: Neighbor update without coupling; Coupling without update; $\frac{1}{2} - \frac{1}{2\sqrt{2}}$ coupling, $\frac{1}{2} + \frac{1}{2\sqrt{2}}$ coupling

RIGHT TOP: Cell count of coupled states and uncoupled states.

RIGHT BOTTOM: Uncoupled states.



Trigonometric Expression of Coupling

$$\cos^2\left({}^{\pi}/_{8}\right) = \frac{1}{2} + \frac{1}{2\sqrt{2}}$$

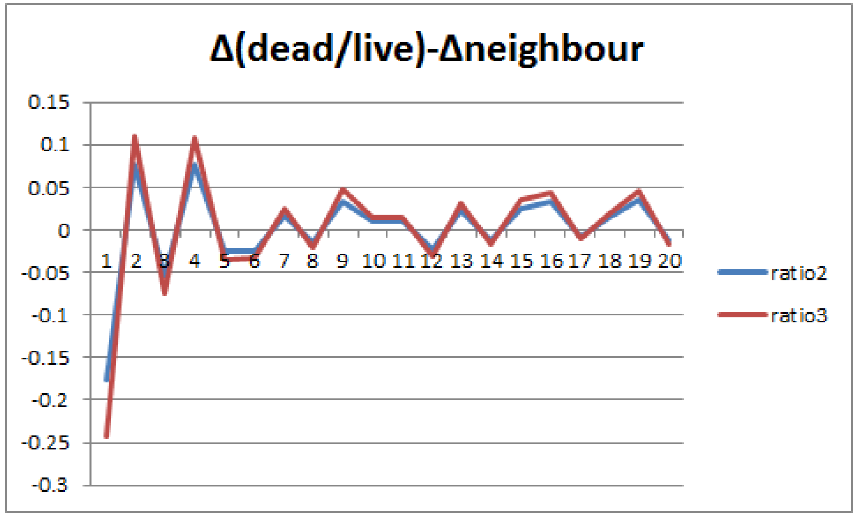
$$\sin^2\left({}^{\pi}/_{8}\right) = \frac{1}{2} - \frac{1}{2\sqrt{2}}$$

$$\cos^2\left({}^{\pi}/_{8}\right) - \sin^2\left({}^{\pi}/_{8}\right) = \frac{1}{\sqrt{2}} = 2\sin\left({}^{\pi}/_{8}\right)\cos\left({}^{\pi}/_{8}\right)$$

General Expression:

$$a\sin^2 x - b\cos^2 x = \sin x \cos x$$

Differential Expression of Coupling



Differential Expression:

$$a \sin^2 x - b \cos^2 x = \sin x \cos x$$

$$\frac{\partial a(b,x)}{\partial b} = \cot^2 x \;;\; \frac{\partial b(a,x)}{\partial a} = \tan^2 x$$

$$\frac{udv}{vdu}$$

$$v = \cos x$$

$$u = \sin x$$

$$\frac{sinx(-\sin x)}{\cos x(\cos x)}$$

$$-tan^2 x$$

5th Rule: 1st Transformation

$$a \sin^2 x - b \cos^2 x = \sin x \cos x$$

when above equation is solved:

$$\therefore b \cot^2 x + \cot x - a = 0$$

when the transformations are applied:

count0 = cell with state 0 count

count1 = cell with state 1 count

j = neighbor count, i = total grid

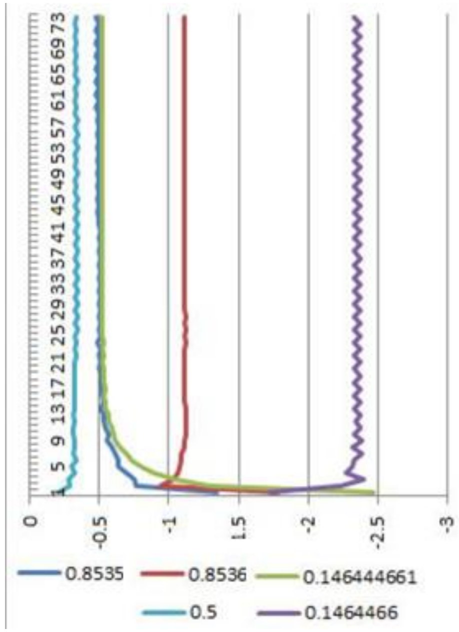
$$\sin x = 8count1$$

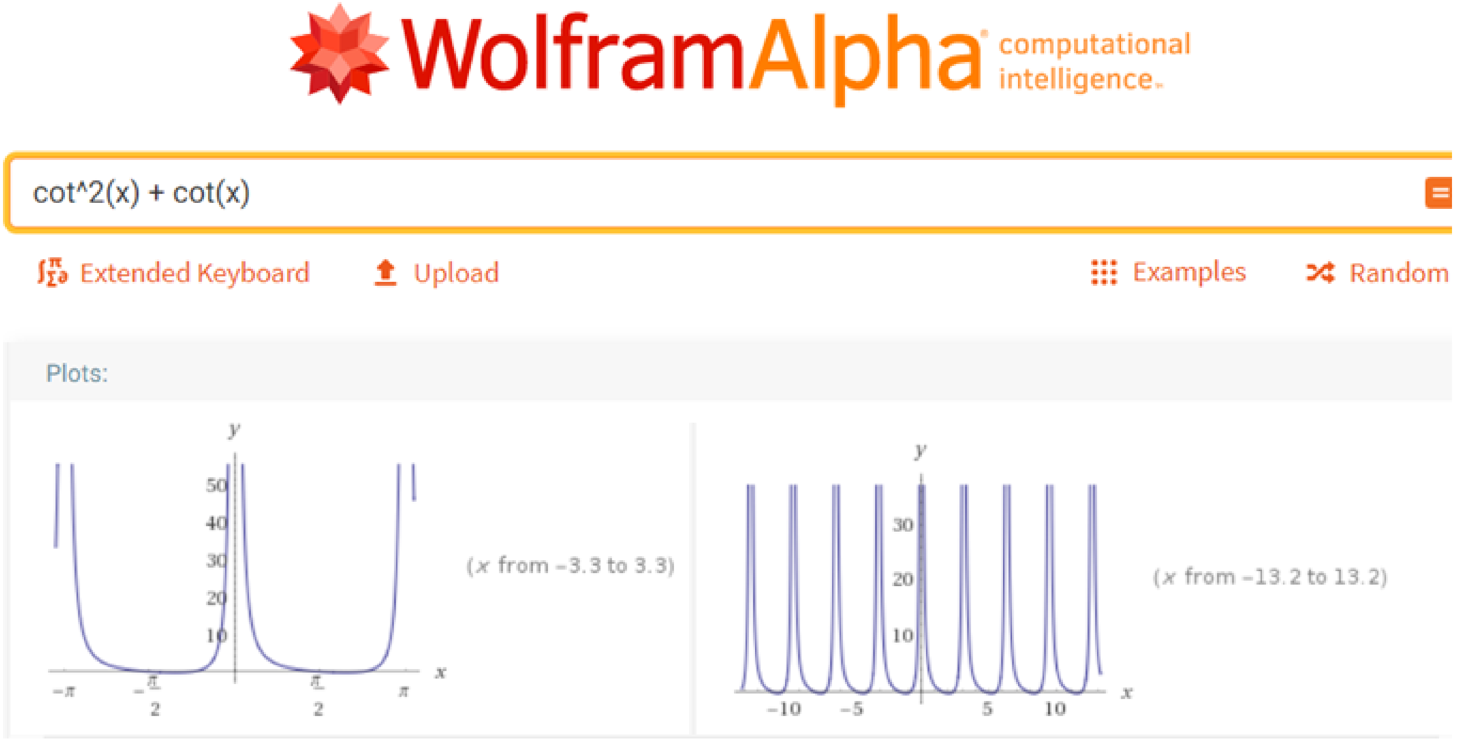
$$\cos x = \frac{count0}{count1}$$

$$-\Delta\frac{j}{i} \times \frac{i^2 \times count0^2}{64 \times count1^4} - \frac{i \times count0}{8 \times count1^2} + \left(\frac{\Delta count0}{\Delta count1}\right)_1 - \left(\frac{\Delta count0}{\Delta count1}\right)_2$$

Cotangent Graph Output of CA

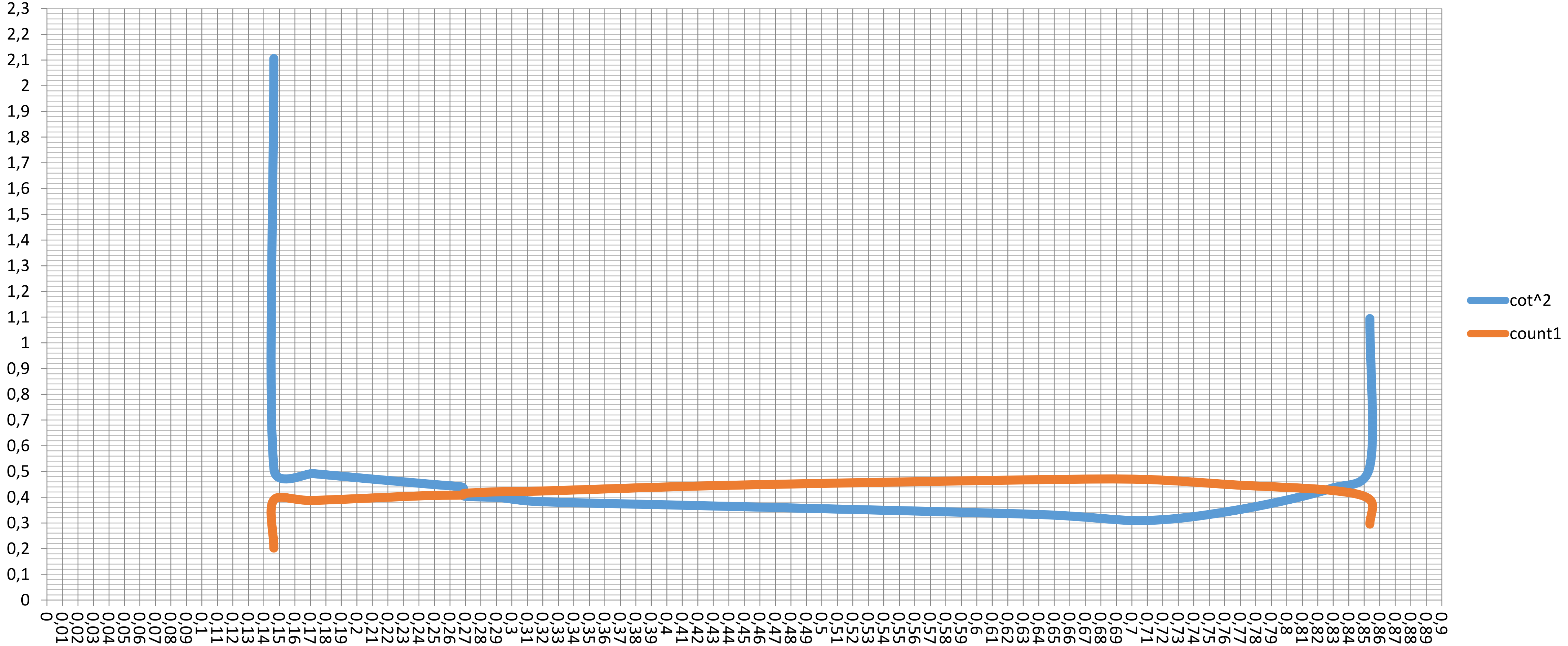
Coupled and uncoupled values are arms of the cotangent graph.





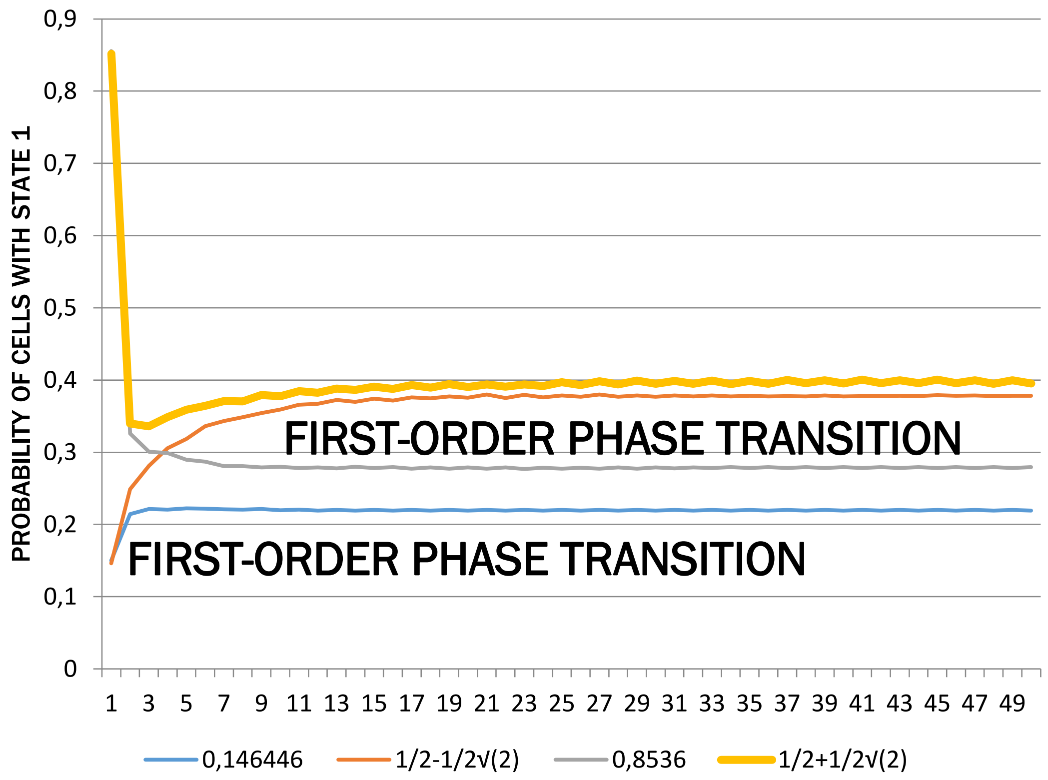
Cotangent & Response Graph Intersection

Intersection points at: $\ln(1+\sqrt{2})/_{2} - \tan^2(\pi/_8)$ and $2\tan(\pi/_8)$



Ferrimagnetic-Ferromagnetic Transition

Lennard-Jones potential **(first-order phase transition – top, bold)**
Ferromagnetic phase **(second-order phase transition)**



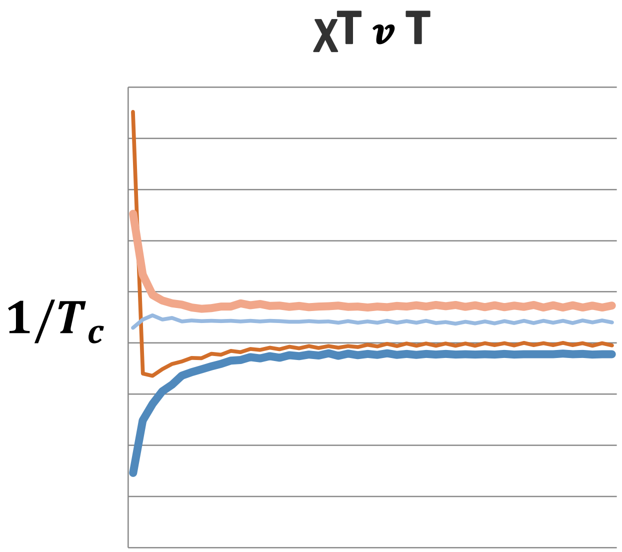
Antiferromagnetic phase
(first-order phase transition - bottom)

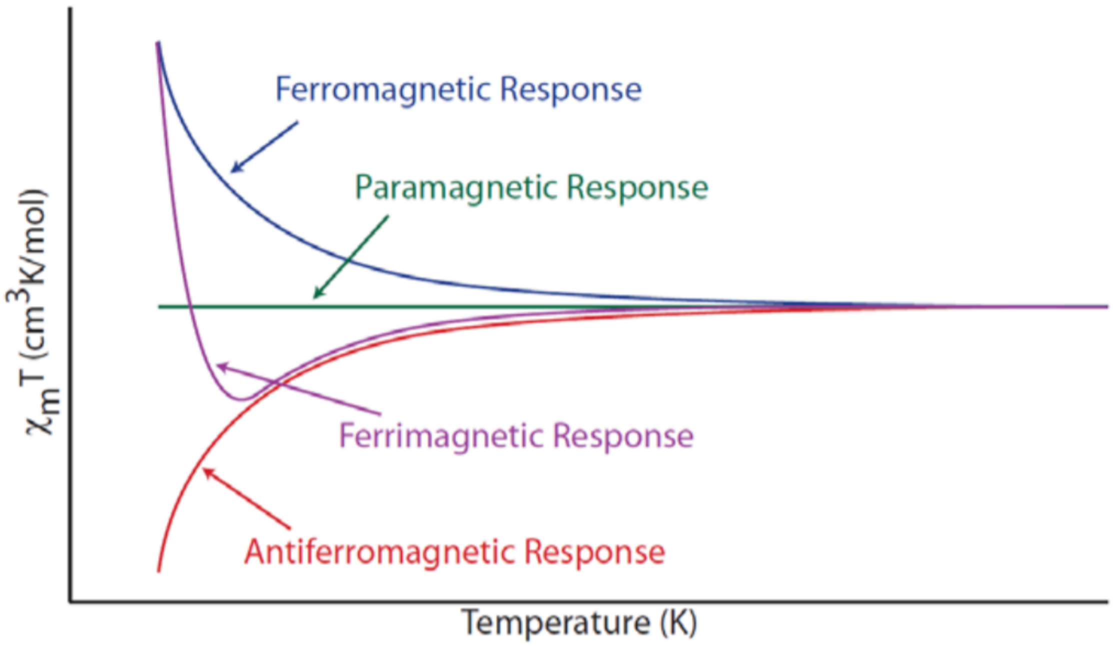
$$p = \frac{1}{2} + \frac{1}{2\sqrt{2}} \approx \mathbf{0.8535; 0.8536}$$

$$p = \frac{1}{2} - \frac{1}{2\sqrt{2}} \approx \mathbf{0.1466; 0.1465}$$

Magnetic Susceptibility v. Temperature

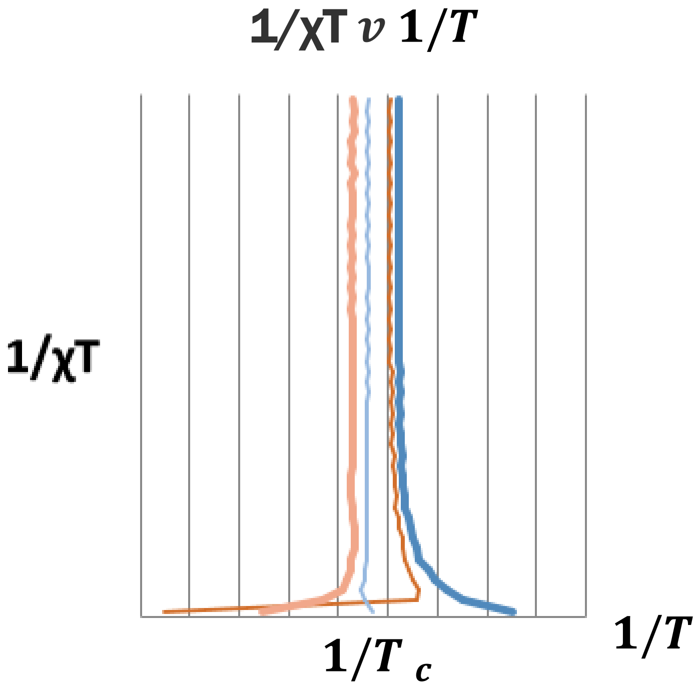
The transition from antiferromagnetic to ferromagnetic phase is very similar to molar magnetic susceptibility to temperature response.

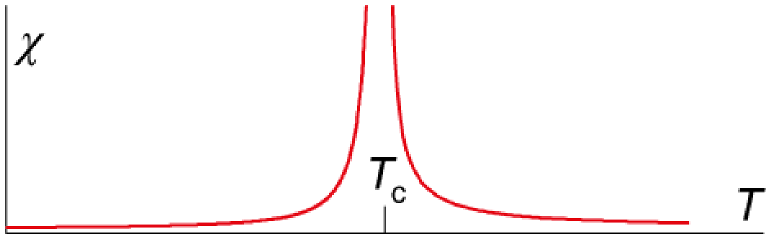




Second-Order Phase Transition

Inverse critical temperature and inverse magnetic susceptibility





SECOND-ORDER PHASE TRANSITION

Symmetry axes of the Magnetic Phases

There are two symmetry axes that correspond to different phases[3].

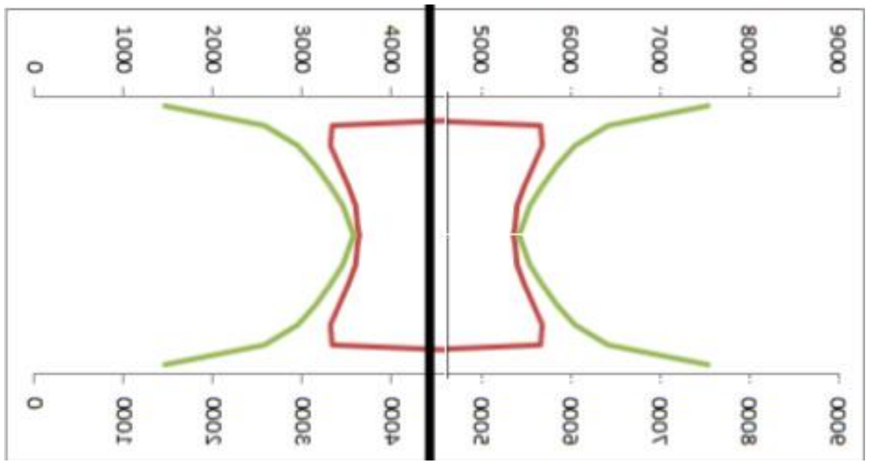


Figure: Catenoid around p = 1/2

FIRST-ORDER
PHASE TRANSITION

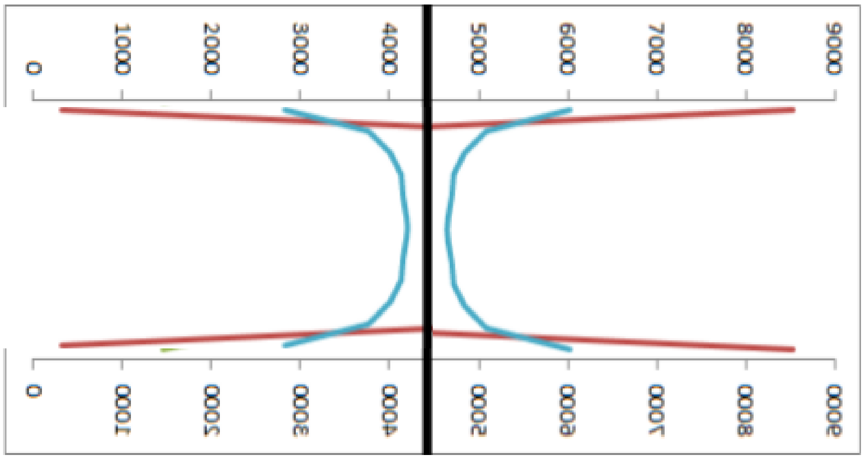


Figure: Pseudosphere around p = ln(1+√2)/2

SECOND-ORDER
PHASE TRANSITION

3. https://www.researchgate.net/publication/348521157_A_2D_Ising_Model_Cellular_Automaton_Mapped_Onto_Catenary_Involute

Ferrimagnetic-Ferromagnetic Transition

The transition point is when the lower bound intersection of cotangent graph and count1 graph is added upon the ½ symmetry.

$$p_{ff} = \frac{1}{2} + \frac{\ln\left(1 + \sqrt{2}\right)}{2} - \tan^2\left(\frac{\pi}{8}\right)$$

Maximum Count1: Evasion Curve

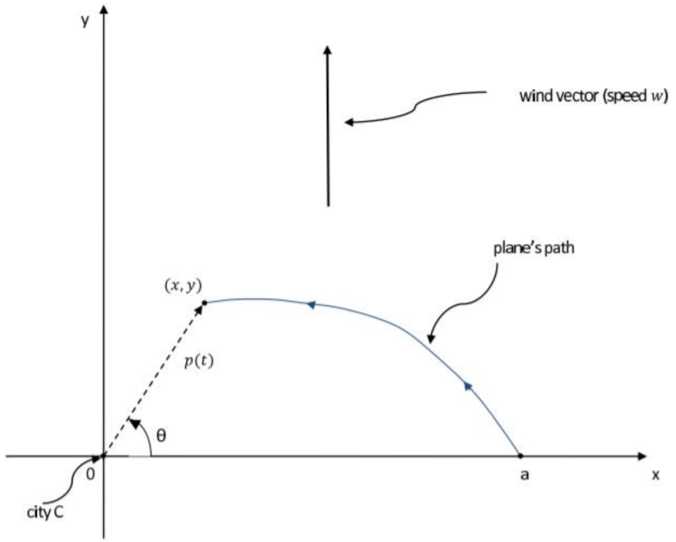


Figure Left. Wind-blown plane problem, longest flight distance under constant wind.

Longest distance is $\approx 1.6478\ for\ a = 1$.

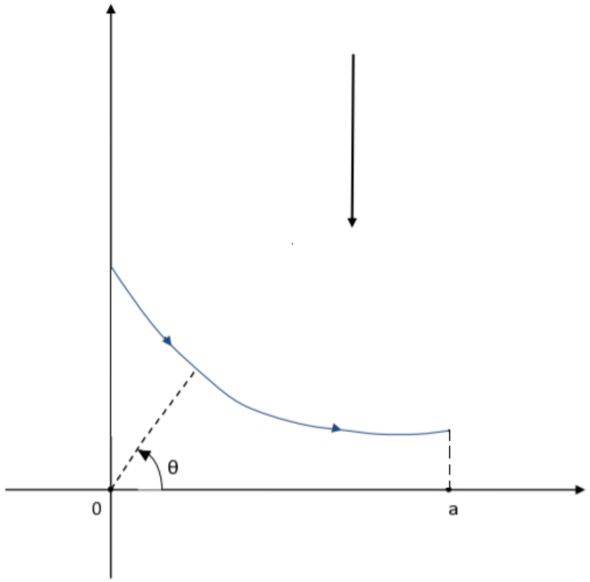


Figure Right. Evasion curve, adapted from the wind-blown plane problem for longest distance away from the inverse Curie temperature.

Highest magnetic susceptibility = $\chi_{MAX} = -\frac{1}{2} + \frac{\ln(1+\sqrt{2})}{2} + \frac{\sqrt{2}}{2}$

$$\chi_{MAX} = \frac{\ln(1+\sqrt{2})}{2} + \frac{\sqrt{2}-1}{2} = \frac{\ln(1+\sqrt{2})}{2} + \frac{\tan{}^{\pi}/_{8}}{2}$$

Left Fig. and problem solution: Nahin, Paul J. Chases and Escapes: The Mathematics of Pursuit and Evasion. Princeton University Press, 2007. JSTOR, www.jstor.org/stable/j.ctt7sbdk.
Right Fig.. Redrawn Image Moiseeva, Svetlana. "Optimal control problems, curves of pursuit." (2011).https://digitalrepository.unm.edu/math_etds/31

Transition Point - Maximum Count1

$$\frac{1}{2} + \frac{\ln\left(1+\sqrt{2}\right)}{2} - \tan^2\left(\frac{\pi}{8}\right) - \frac{\ln\left(1+\sqrt{2}\right)}{2} - \frac{\tan {}^{\pi}/_{8}}{2}$$

which is simplified to:

$$-\frac{1}{2}\left(2\cot^2\left(\frac{3\pi}{8}\right) + \cot\frac{3\pi}{8} - 1\right)$$

This is the cotangent equation we have derived before:

$$\therefore b\cot^2 x + \cot x - a = 0$$

Its root is $x = \tan^{-1}({}^{1}/_{2}) \approx 0.46\,365$

Renormalization Recursion

$0.46365 \approx 0.4656665$

Recursion equation:

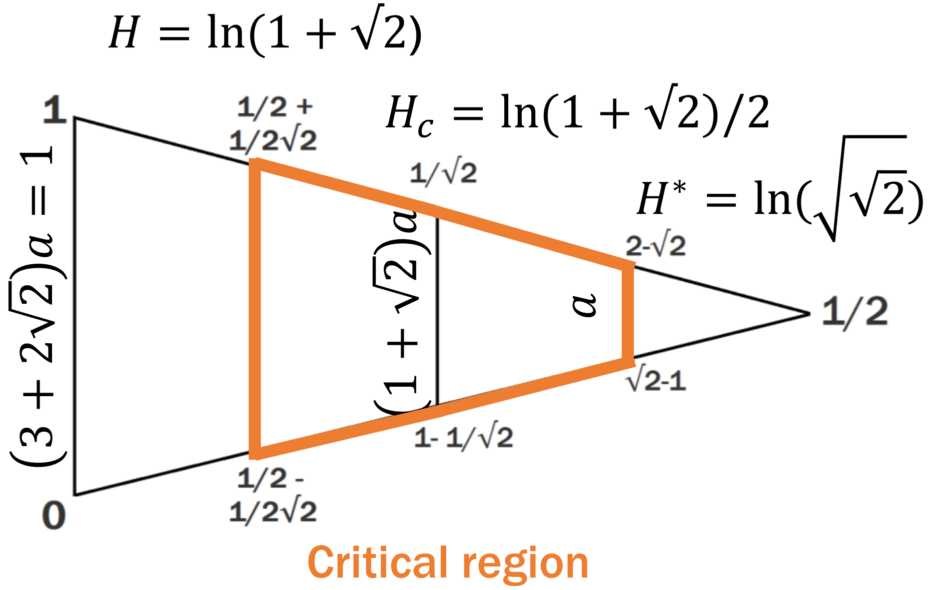
$\cos(2\tan^{-1} 0.4656665)$

When ran sequentially,

the recursion returns

H, H_c and H* magnetic fields.

This affirms our hypothesis.



2nd Transformation

$count1 = \cos y$

$count0 = \sin y$

When applied to:

$$-\Delta\frac{j}{i} \times \frac{i^2 \times count0^2}{64 \times count1^4} - \frac{i \times count0}{8 \times count1^2} + \left(\frac{\Delta count0}{\Delta count1}\right)_1 - \left(\frac{\Delta count0}{\Delta count1}\right)_2$$

simplifies to:

$$\frac{1}{\cos^2 y}\left(\frac{1}{8}\tan y \sec y - 1\right) = 0$$

Deriving Cotangent Outputs of CA

- $\boldsymbol{\frac{1}{8}\tan y \sec y - 1 \approx 0.5050}$ is the $p = \frac{1}{2} \pm \frac{1}{2\sqrt{2}}$ output.
- $\boldsymbol{\frac{1}{\cos^2 y}\left(\frac{1}{8}\tan y \sec y - 1\right) \approx 2.269 \approx \frac{2}{\ln(1+\sqrt{2})}}$ is the $\left(p = \frac{1}{2} - \frac{1}{2\sqrt{2}}\right)_-$ output.
- **1** is the $\left(p = \frac{1}{2} + \frac{1}{2\sqrt{2}}\right)_+$ output (demagnetization).

Susceptibility – Curie Law

$\chi = \frac{c}{T \pm \theta} = \frac{1}{4 \pm 2\sqrt{2}}$ for ferrimagnetism and antiferromagnetism

$\chi = \frac{c}{T_c} = \frac{\ln\left(1+\sqrt{2}\right)}{2}$ for paramagnetism

$\chi = \frac{c}{T_f} = \frac{\ln\left(1+\sqrt{2}\right)}{2} + \frac{\tan\left(\frac{\pi}{8}\right)}{2}$ for global maximum of ferromagnetism

THANK YOU FOR LISTENING!

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https://github.com/goktu/ADama/blob/master/cellularautomata.py