Project 2: Random Processes & Complex Systems

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2.1: Polymers as Random 2D Walks

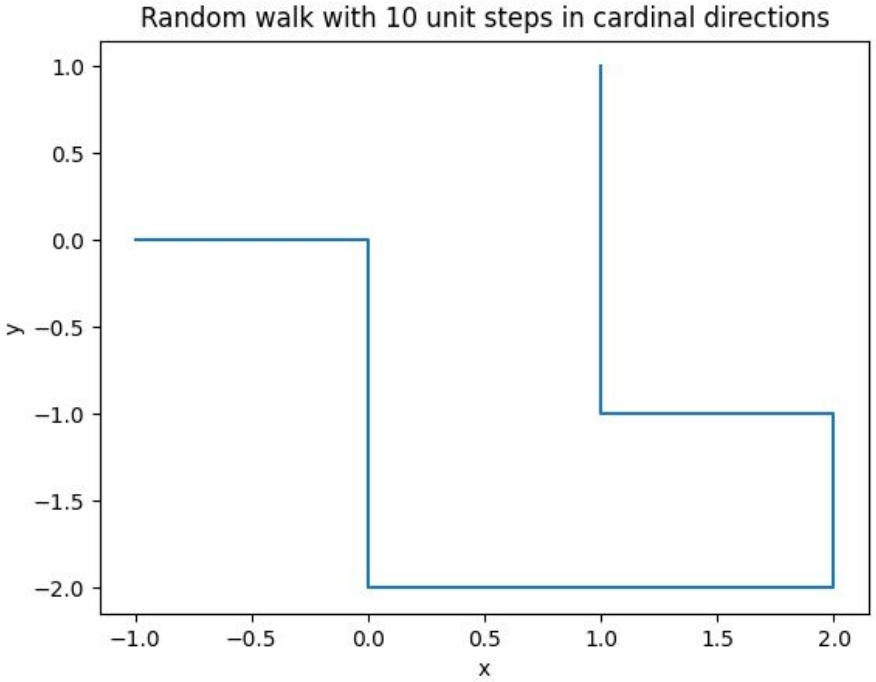
Organic polymers

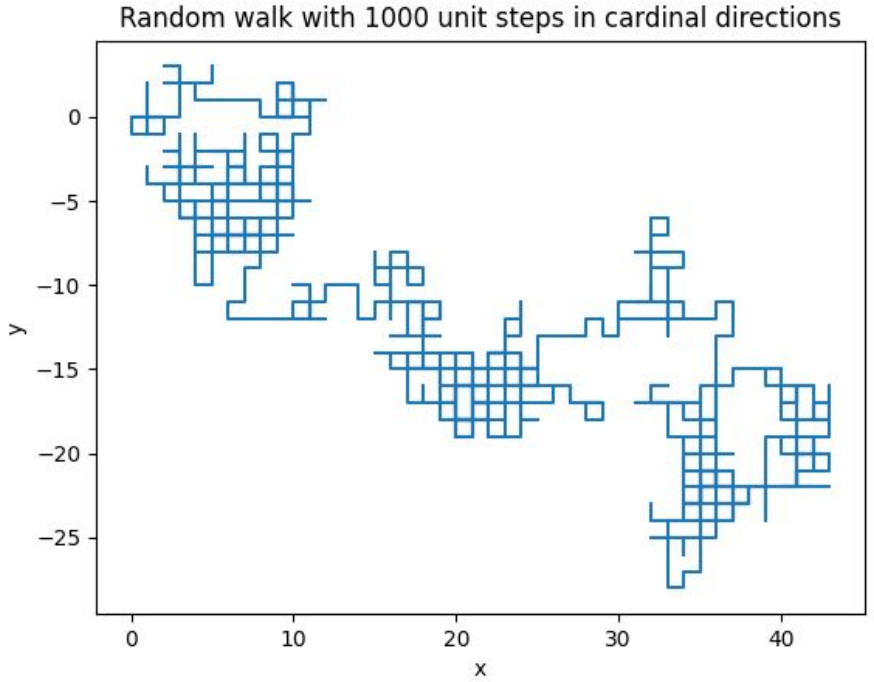
Approximation and simulation using mathematical random walks

What's a random walk?

- Discrete: single/unit steps
- Steps in cardinal directions

Part a)


Random walk with 10 unit steps in cardinal directions
1.0
0.5
0.0
−0.5
−1.0
−1.5
−2.0
y
−1.0
−0.5
0.0
0.5
1.0
1.5
2.0
x


Random walk with 1000 unit steps in cardinal directions
0
−5
−10
−15
−20
−25
y
0
10
20
30
40
x

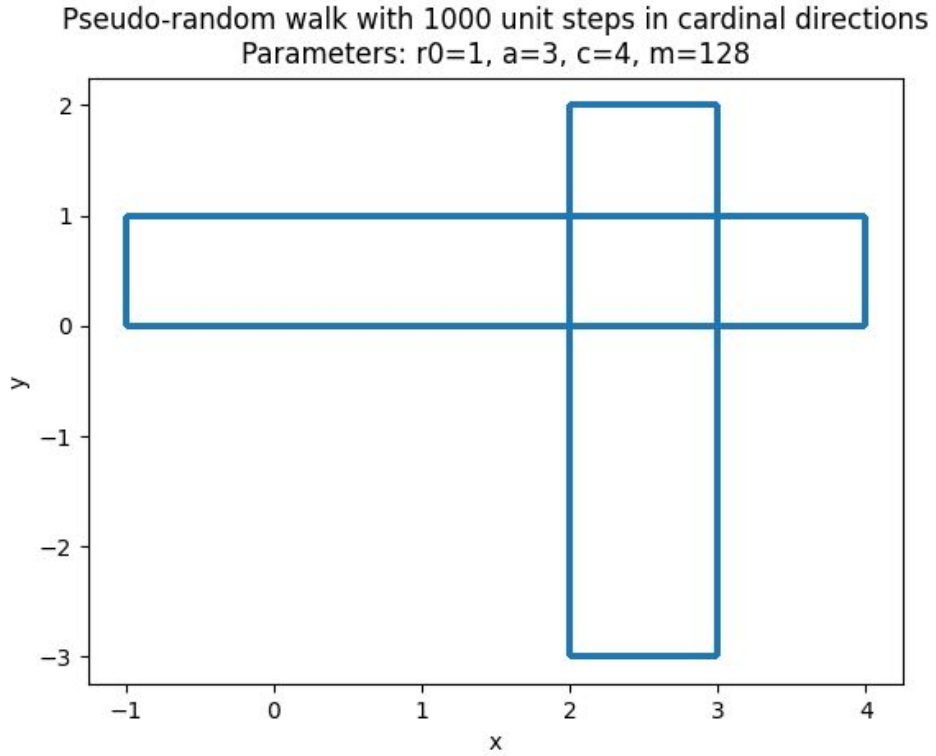
Part b)

Custom RNG

r(n) = (a * r(n-1) + c) mod m

Default:

r(0) = 1, a = 3, c = 4, m = 128



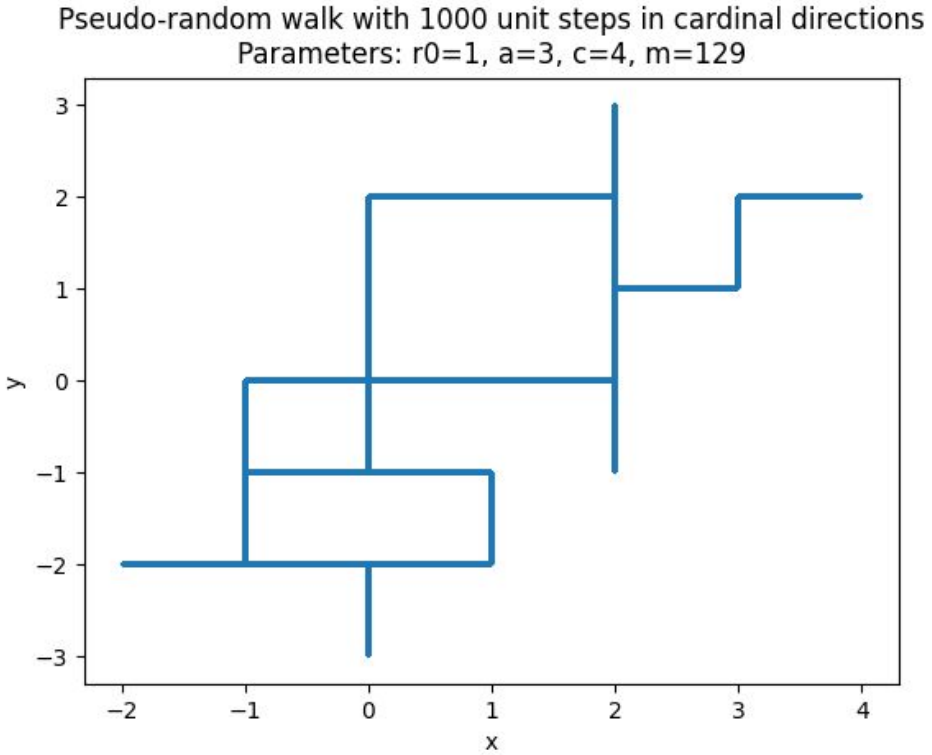
Part b)

Other parameters

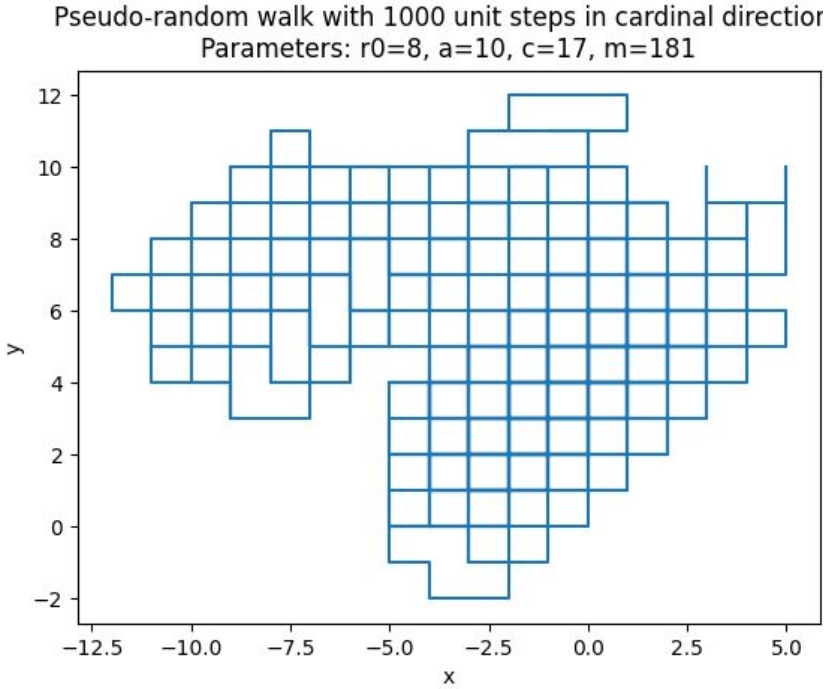
m = 129 (Shown on the right)

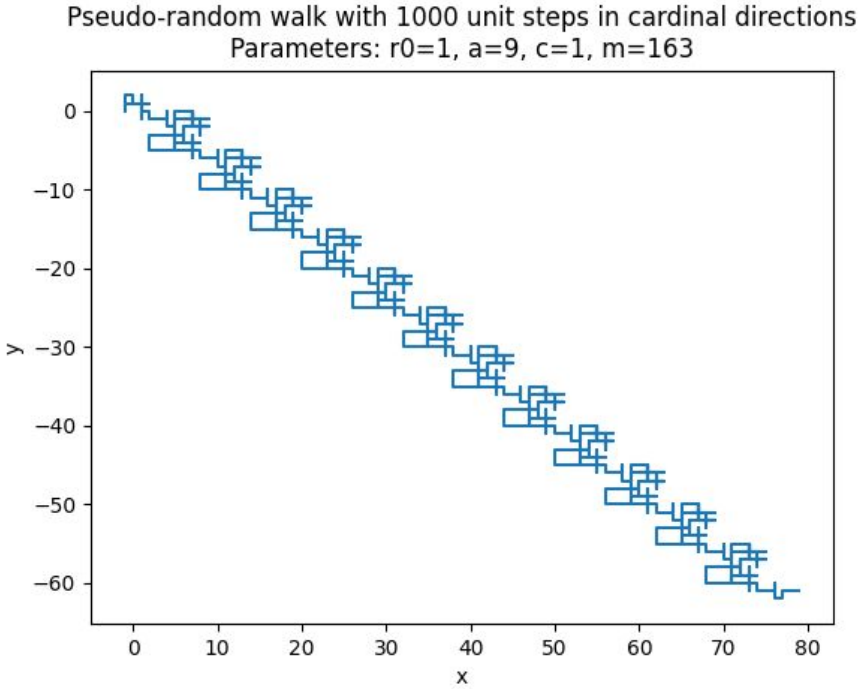
Still *highly* periodic

Random parameters?



Part b)


Pseudo-random walk with 1000 unit steps in cardinal directior
Parameters: r0=8, a=10, c=17, m=181
12
10
8
6
4
2
0
−2
y
−12.5
−10.0
−7.5
−5.0
−2.5
0.0
2.5
5.0
x


Pseudo-random walk with 1000 unit steps in cardinal directions
Parameters: r0=1, a=9, c=1, m=163
0
−10
−20
−30
−40
−50
−60
y
0
10
20
30
40
50
60
70
80
x

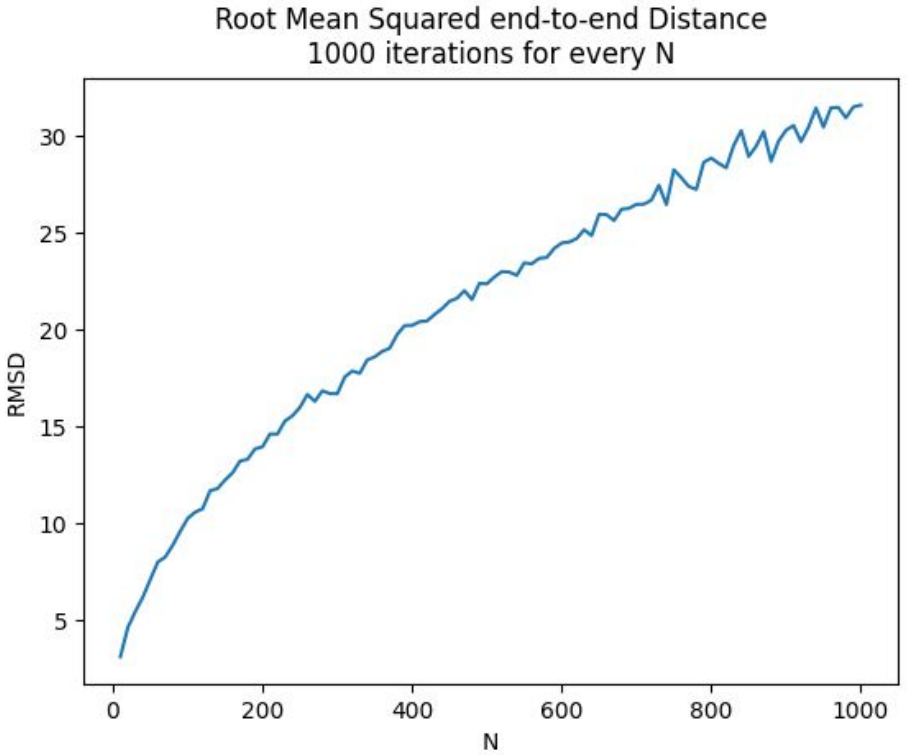
Part c)

Analysis

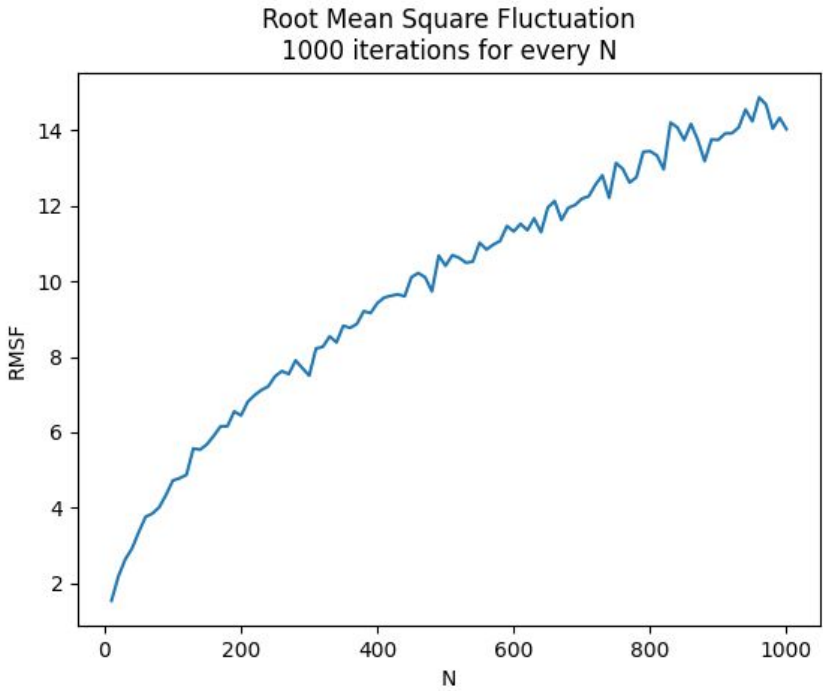
Root mean square end-to-end distance RMSD

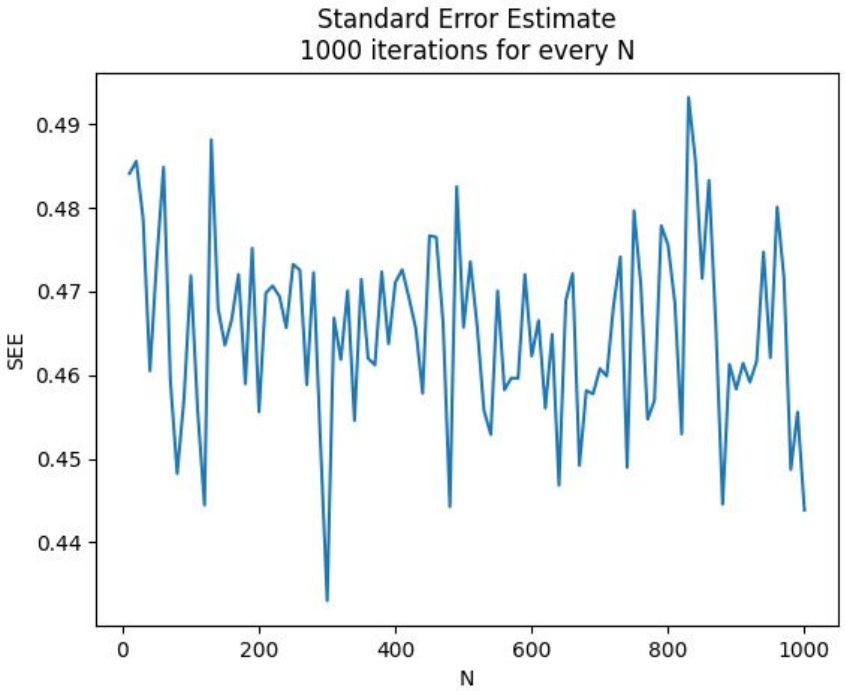
Root mean square fluctuation RMSF

Standard Error Estimate SEE



Part c)


Root Mean Square Fluctuation
1000 iterations for every N
RMSF
N
2
4
6
8
10
12
14
0
200
400
600
800
1000

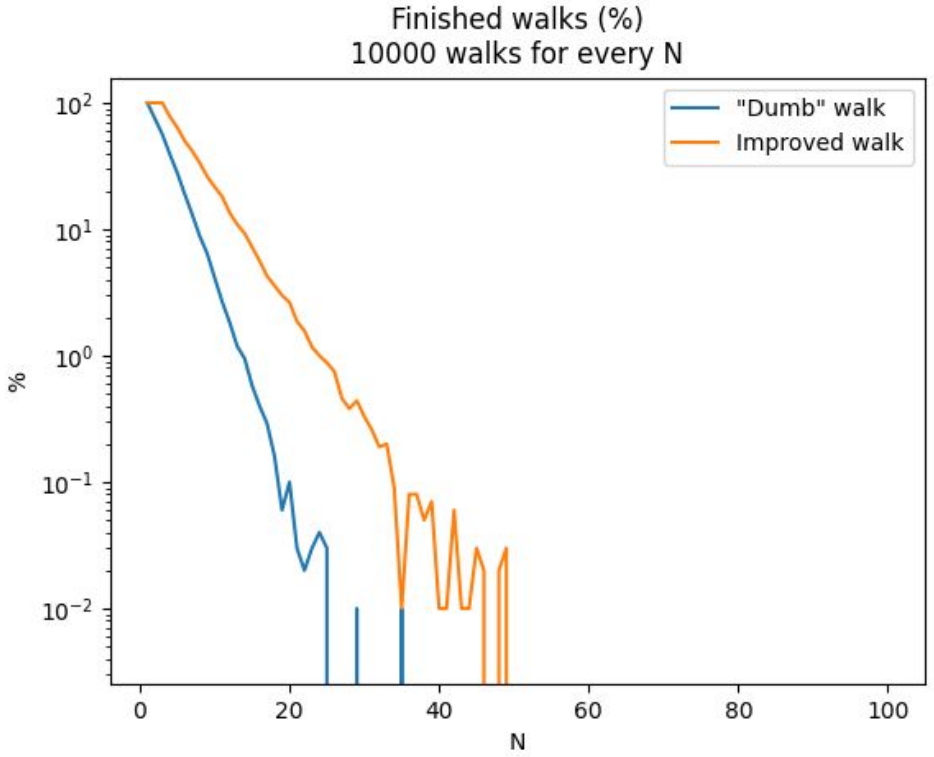

Standard Error Estimate
1000 iterations for every N
SEE
N
0.44
0.45
0.46
0.47
0.48
0.49
0
200
400
600
800
1000

Part d)

Self avoiding walk

Real polymers cannot self intersect: Self avoiding walk

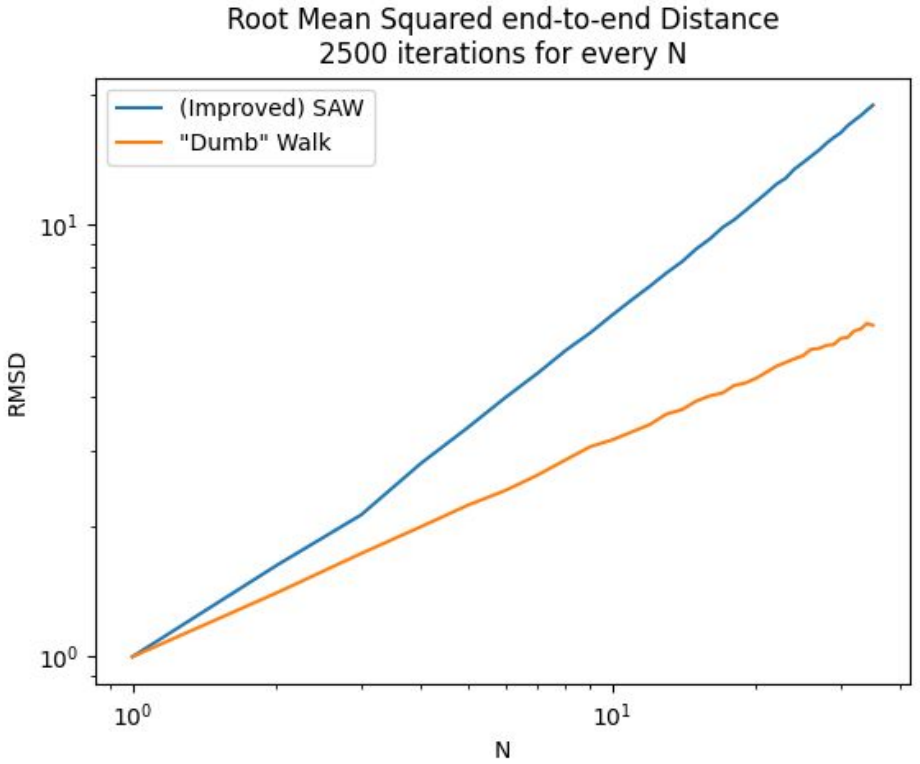
- Discard walk if it self intersects
- Improvement: allow only left, right, and straight ahead
- N = 35 reasonable limit



Part e)

RMSD for SAW

- Close to linear
- “Dumb” walk close to sqrt



2.2: Traffic Model using Cellular Automata

Simulating car traffic

- Cars driving on long road

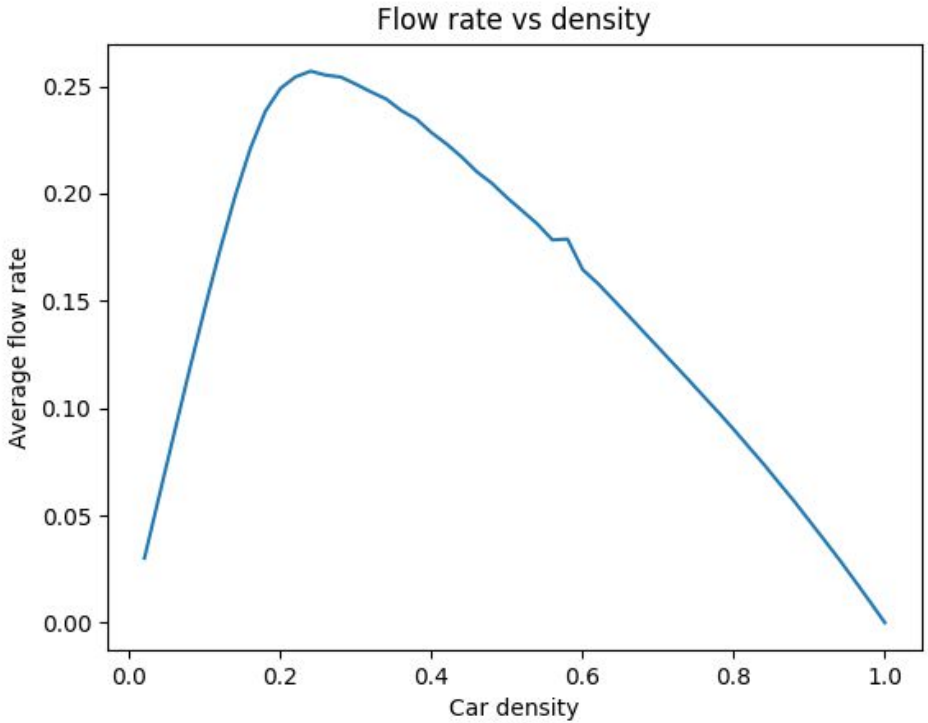
Cellular automata

- Discrete: next state is completely determined by current state
- Periodic boundary conditions
- Simple set of rules that every “cell” obeys

Part a)

Fundamental diagram

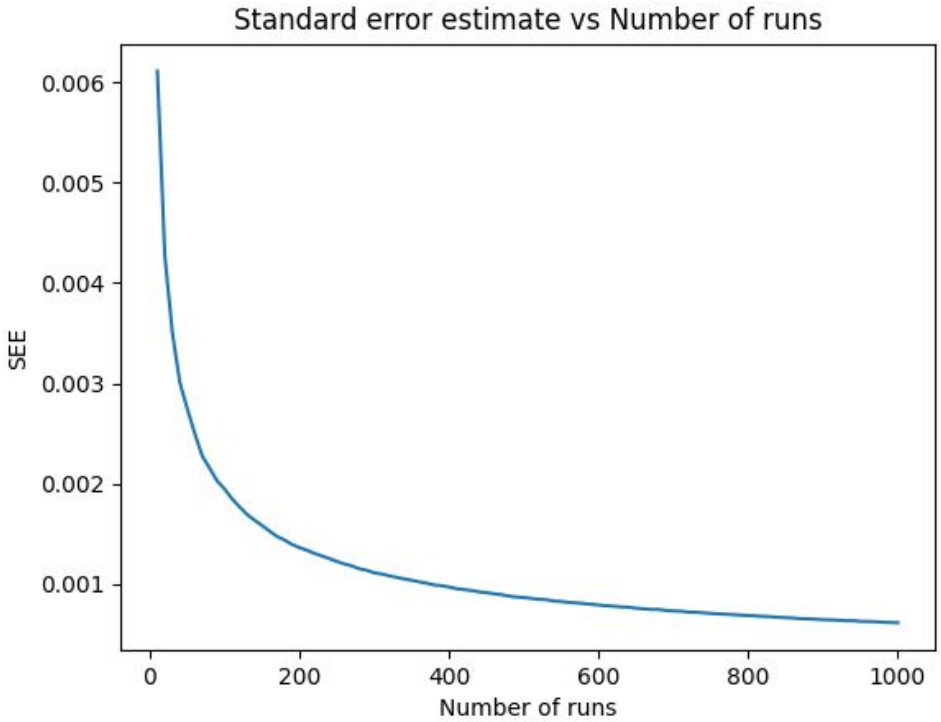
- v_max = 2, p = 0.5
- Plot average flow rate vs car density



Part b)

Statistical accuracy

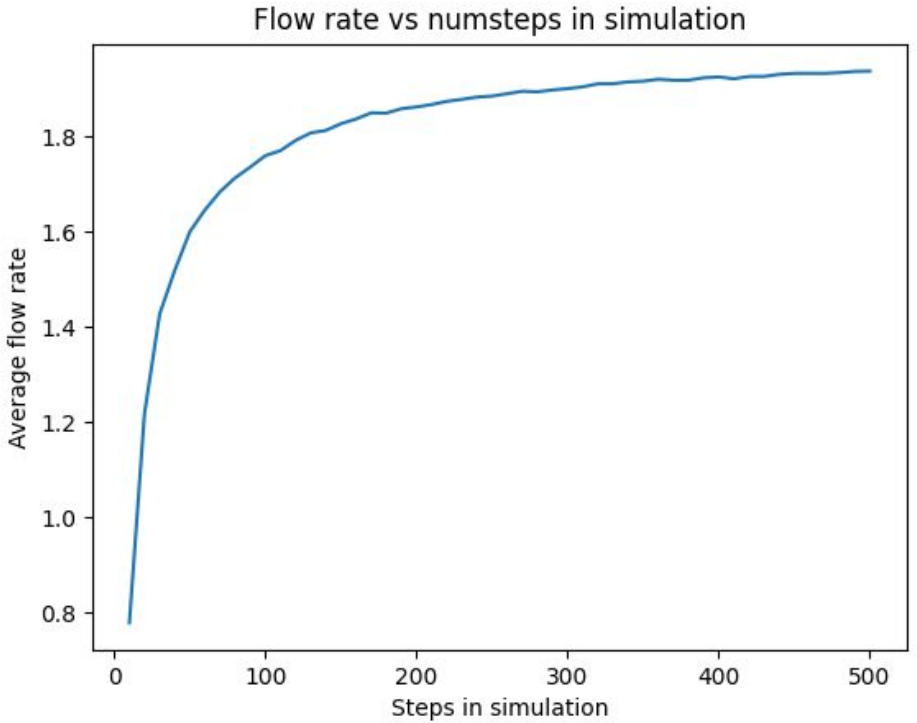
- Standard error estimate
- N = 380 => SEE < 0.001



Part b)

Equilibration time

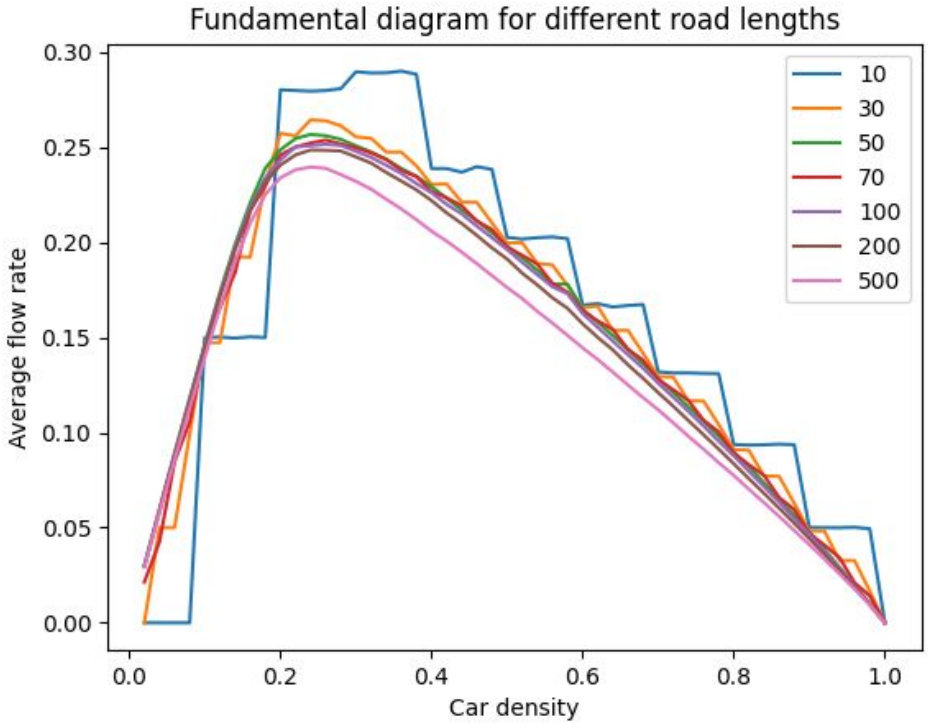
- Standard error estimate
- *All* values of AFR sampled, including during equilibration period
- If only sampling equilibrium, N = 100 might be feasible
- N >= 200



Part c)

System size independence

- Fundamental diagram for multiple road lengths
- By a road length of >= 50, the diagram stops changing
- Integer rounding



Part d) and e)

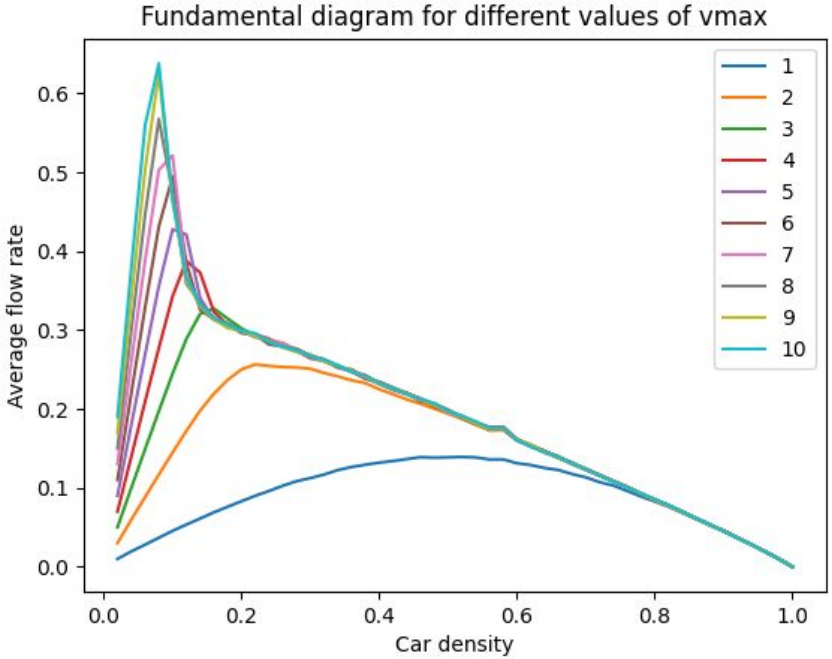
Parameter tinkering

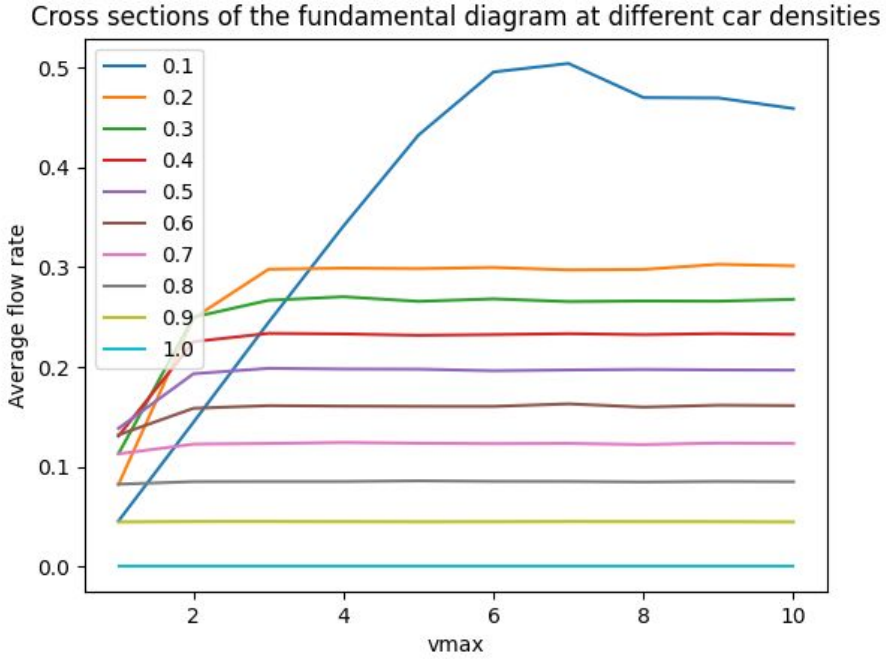
- Varying v_max (d) and p (e)
- Quantitative differences

What's about to come

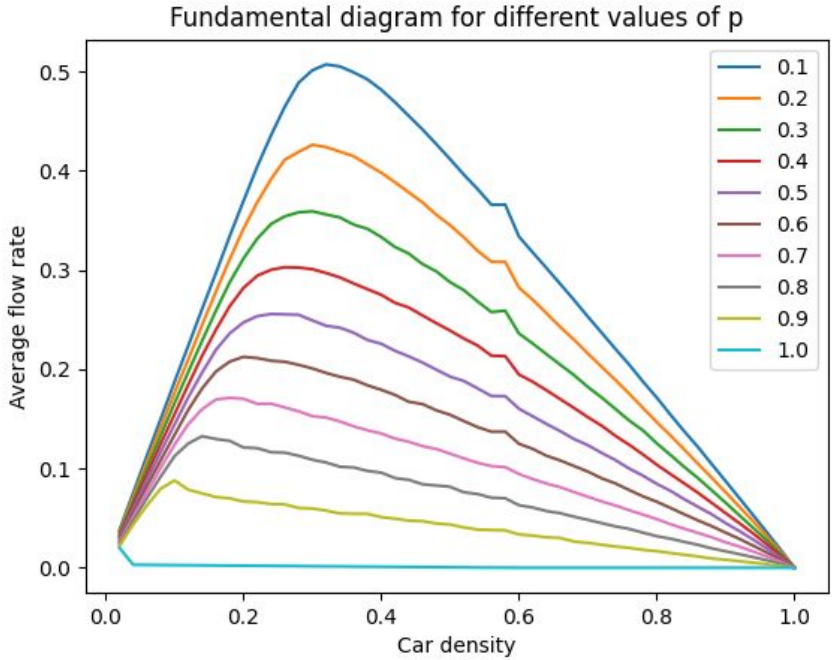
- Fundamental diagrams for different v_max and p
- Cross sections at different car densities

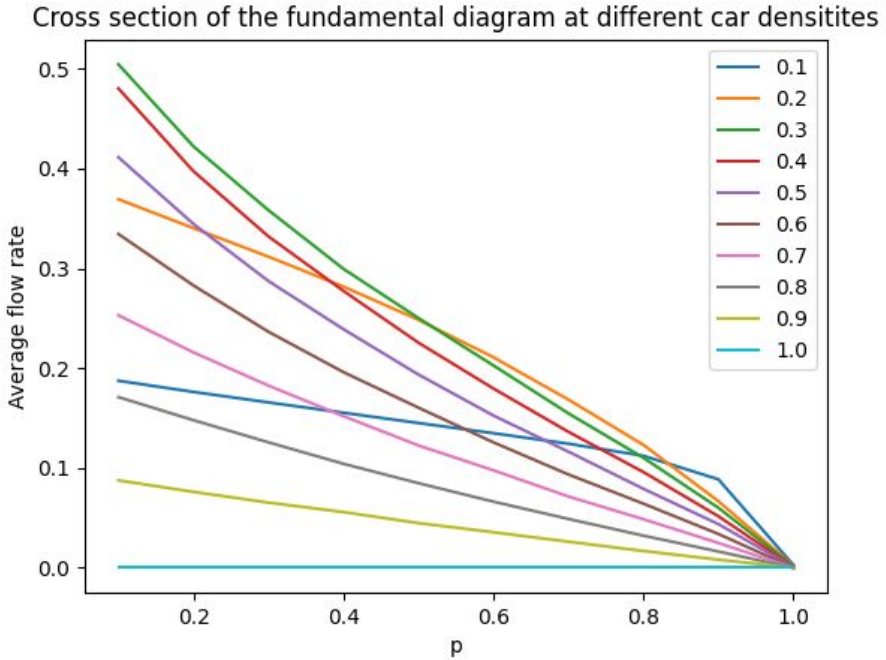
Part d)


Fundamental diagram for different values of vmax
Average flow rate
Car density
0.0
0.1
0.2
0.3
0.4
0.5
0.6
0.0
0.2
0.4
0.6
0.8
1.0
1
2
3
4
5
6
7
8
9
10


Cross sections of the fundamental diagram at different car densities
Average flow rate
vmax
0.0
0.1
0.2
0.3
0.4
0.5
2
4
6
8
10
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1.0

Part e)


Fundamental diagram for different values of p
Average flow rate
Car density
0.0
0.1
0.2
0.3
0.4
0.5
0.6
0.8
1.0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1.0


Cross section of the fundamental diagram at different car densitites
Average flow rate
p
0.0
0.1
0.2
0.3
0.4
0.5
0.6
0.8
1.0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1.0

Thank you!