Endless self-avoiding walks

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Guttmann 2025 - 80 and (still) counting
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A few words about Tony Guttmann

Tony has published about 320 articles and is still going strong.

Tony completed the Annecy Lake Marathon in April, 2025, at age 80.

Tony has made important/central contributions to AMSI, MASCOS, ANZAMP, MATRIX, ACEMS, and probably many more things I don't know about. In recognition of this the prize for the best student talk at the ANZAMP meeting is called the Guttmann Prize.

Tony has won many awards, some are

- Fellow, Australian Academy of Science
- Fellow Australian Academy of Technological Sciences and Engineering
- Member of the Order of Australia (AM) for significant service to the mathematical sciences, and to education
- See: https://www.eoas.info/biogs/P007187b.htm

A few words about Tony Guttmann

Tony is a natural community builder who has made the mathematics and mathematical physics communities stronger.

Tony does things right: creative/fun/interesting/important research, builds communities, helps younger scientists, and enjoys life.

To Tony, thank you for being an inspiration, and for your help and guidance over the years since I started as a research fellow in MASCOS, 139 Barry St, back in 2004.

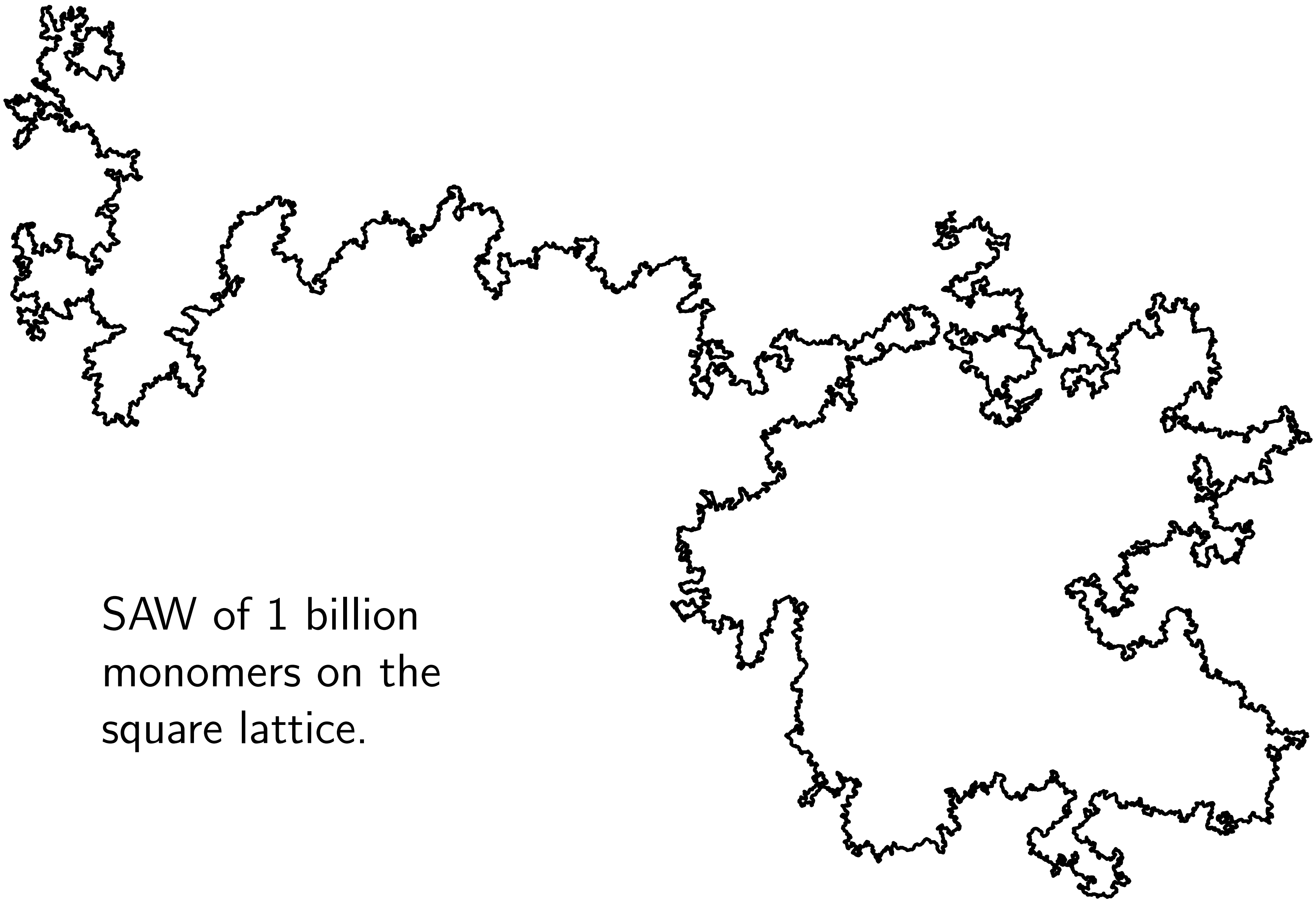
Happy birthday Tony!

This work has been done in collaboration with Neal Madras.

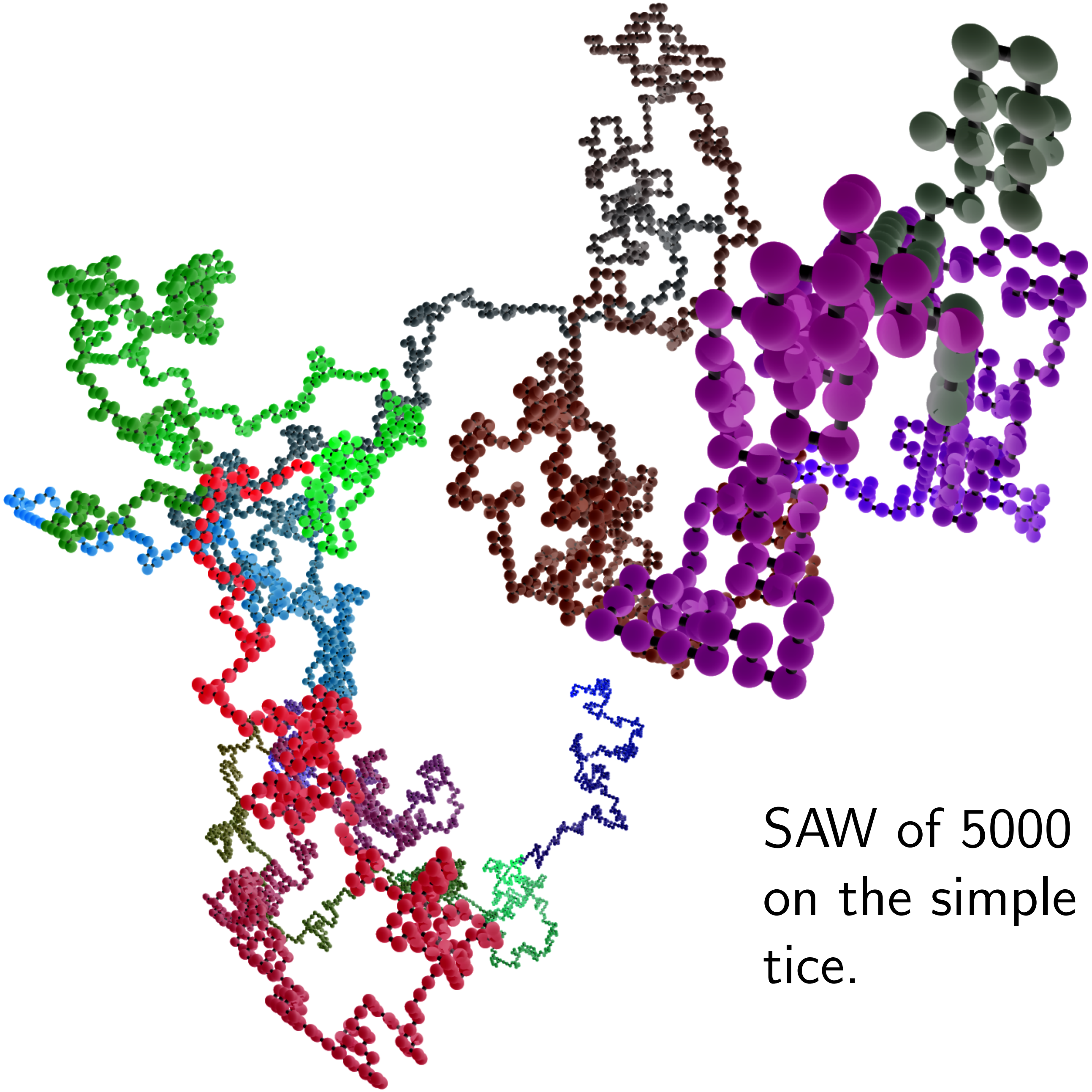
From Neal: Happy birthday, Tony!

Self-avoiding walk model

- A walk on a lattice, step to neighbouring site provided it has not already been visited.
- Captures excluded volume effect of real polymers.
- Models polymers in good solvent limit.
- Exactly captures universal properties such as critical exponents.
- Generalisations allow study of a wide range of polymer systems, e.g. the collapse transition, or polymer melts.



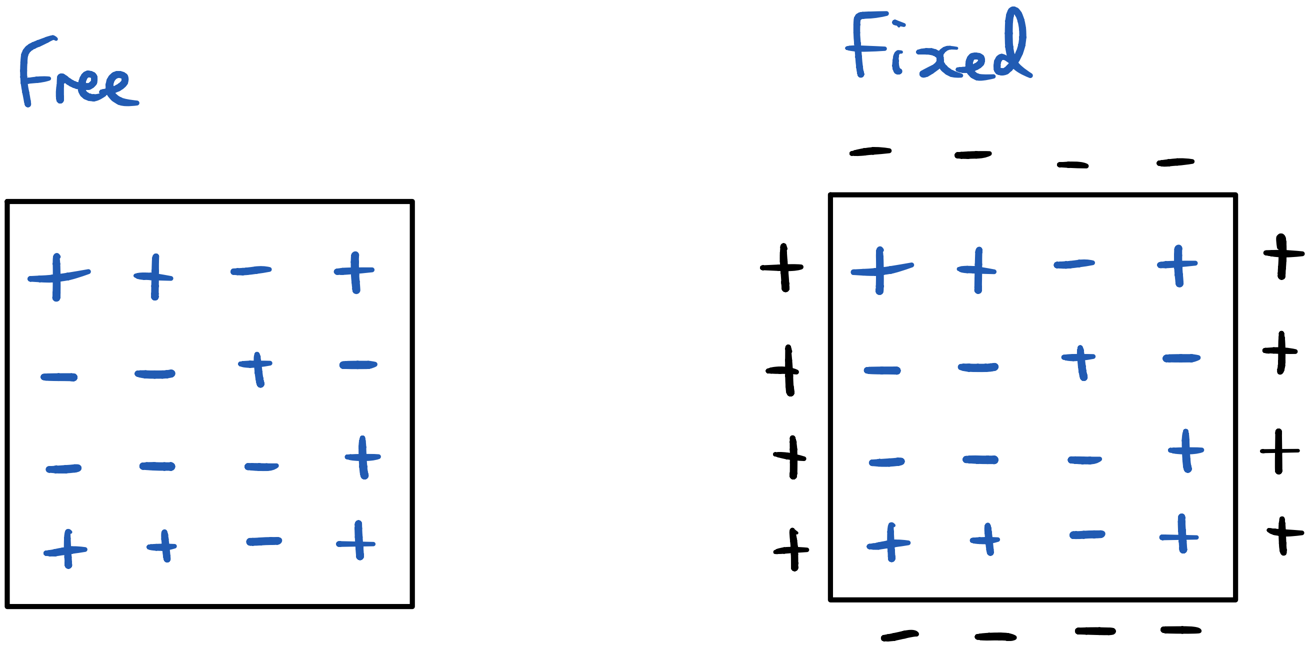
SAW of 1 billion monomers on the square lattice.



SAW of 5000 monomers on the simple cubic lattice.

Why endless walks?

For spin models we have a natural choice between boundary conditions

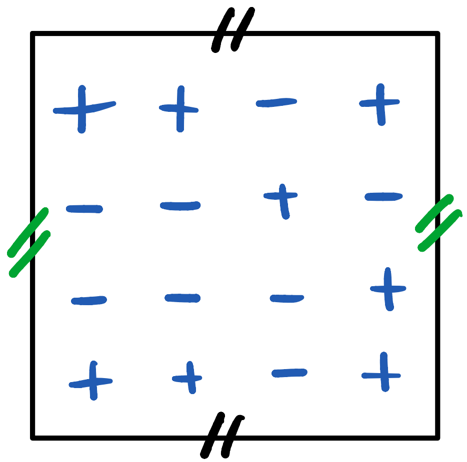


Free and fixed BCs have an internal length scale: distance to boundary

Why endless walks?

For periodic boundary conditions (PBC) we have translation invariance

Periodic:



Why endless walks?

For periodic boundary conditions (PBC) we have translation invariance

Periodic:

+	+	−	+
−	−	+	−
−	−	−	+
+	+	−	+

Why endless walks?

For periodic boundary conditions (PBC) we have translation invariance

Periodic:

+	+	−	+	+	+	−	+	+	+	−	+
−	−	+	−	−	−	+	−	−	−	+	−
−	−	−	+	−	−	−	+	−	−	−	+
+	+	−	+	+	+	−	+	+	+	−	+
+	+	−	+	+	+	−	+	+	+	−	+
−	−	+	−	−	−	+	−	−	−	+	−
−	−	−	+	−	−	−	+	−	−	−	+
+	+	−	+	+	+	−	+	+	+	−	+

Why endless walks?

We can consider system with PBC as being 'infinite' with no boundary.
(Although the box size L is still a natural length scale.)

Why endless walks?

How about walks?

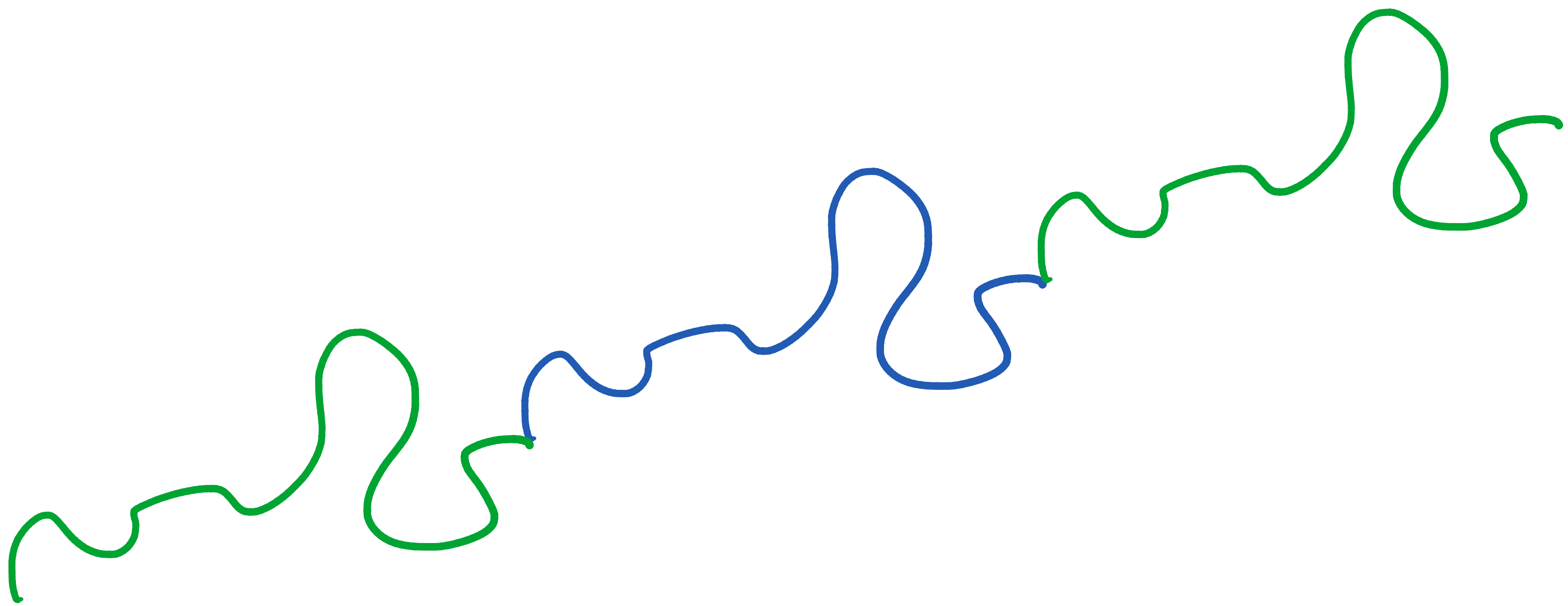
They are easy to define on an infinite lattice or $\mathbb{R}^d$, so are translationally invariant.

<u>But</u>, interior of walk is different from ends

For a self-avoiding walk (SAW):

Why endless walks?

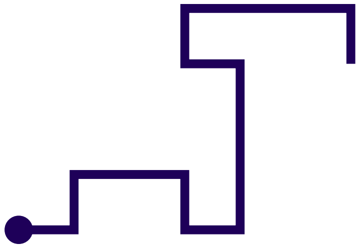
Idea : PBC with respect to <u>chain</u> (not space)



Endless walks

- Consider walks which are concatenated with themselves ad infinitum, where infinite walk satisfies same rule as reduced walk.
- E.g. endless self-avoiding walks (SAWs) remain self-avoiding when concatenated with themselves.
- Motivation:
  - Eliminate end-effects, improve convergence to infinite chain.
  - Possibility for other nice properties.

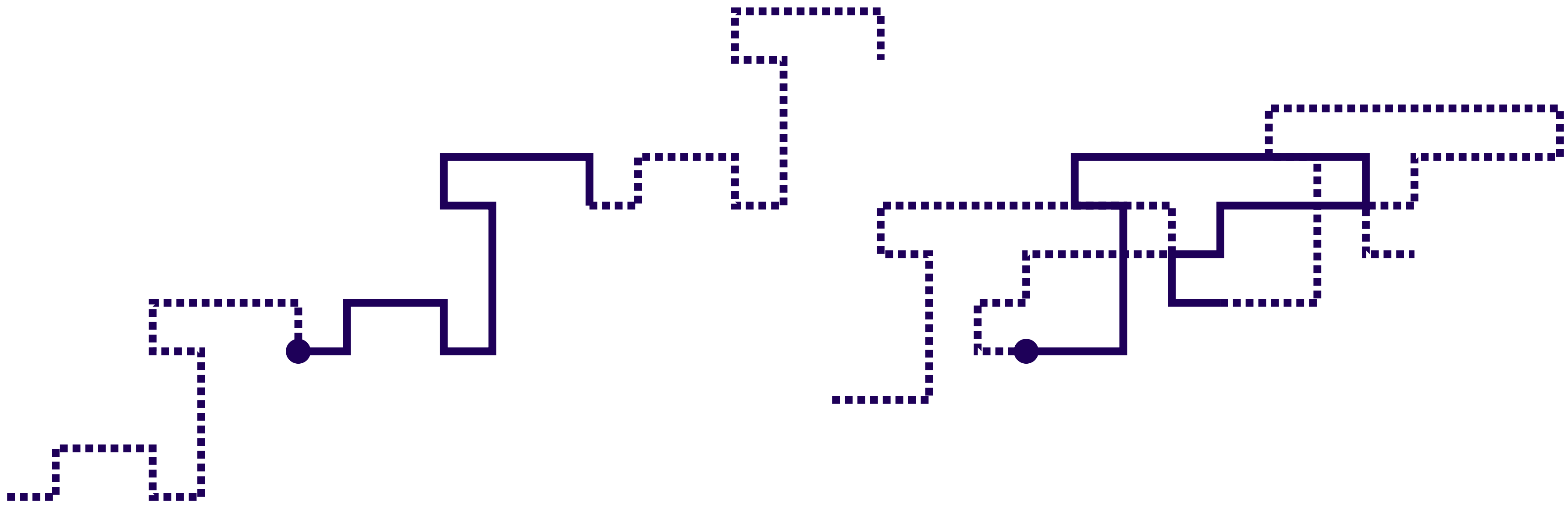
Examples



endless SAW

SAW that is not endless

Examples



endless SAW

SAW that is not endless

Endless SAWs

- Assume that $e_n = A_e n^{\gamma_e - 1} \mu^n (1 + o(1))$.
- Same μ as SAWs (proved).
- $\gamma_e = 1$ (hand-waving, numerical evidence; Neal Madras: argument that $\gamma_e \geq 1$ provided that critical exponent exists for bridges).
- Universal amplitude A_e, dependent on dimension but not lattice (hand-waving, numerical evidence from enumerations).
- Enumeration data from 2013: $A_e = 1.57075(10)$ for $d = 2$, and $A_e = 1.183(3)$ for $d = 3$.

Transfer matrix

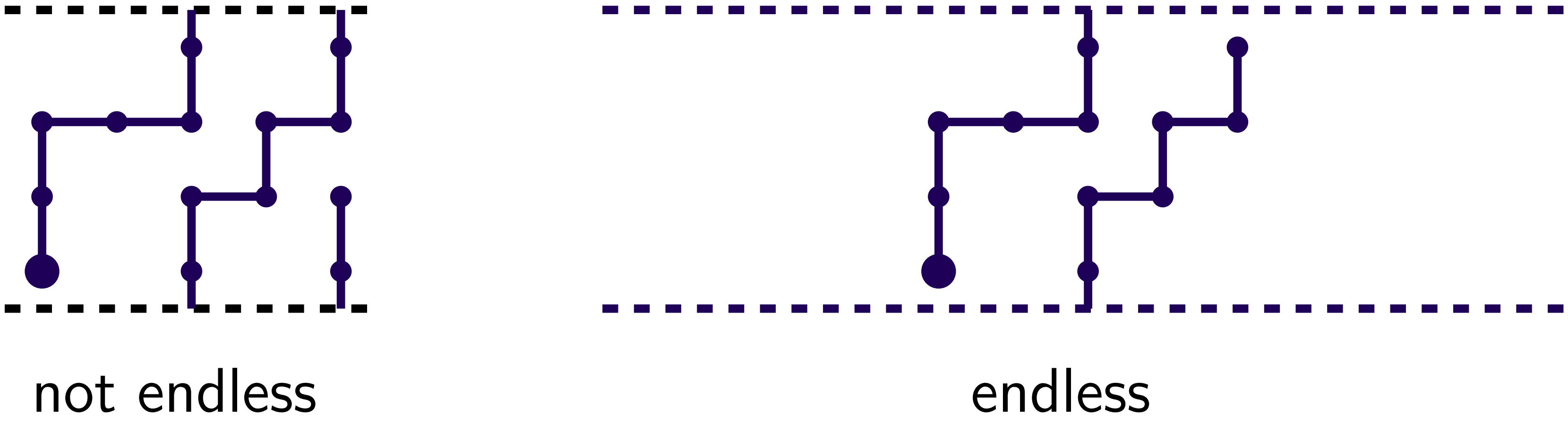
- Suppose model has a finite state space, and hence a finite transfer matrix.
- Then, endless walks are the subset of walks which end in the same state as they started.
- Number of endless walks of length n

$$e_n = \sum_x \langle x| T^n |x\rangle = \mathrm{Tr}\, T^n = \lambda_1^n + \cdots + \lambda_k^n,$$

  i.e. sum of exponentials with unit amplitude.
- Generically, generating function

$$E(z) = \sum_{n\geq 1} e_n z^n = \frac{\lambda_1 z}{1-\lambda_1 z} + \cdots + \frac{\lambda_k z}{1-\lambda_k z}.$$

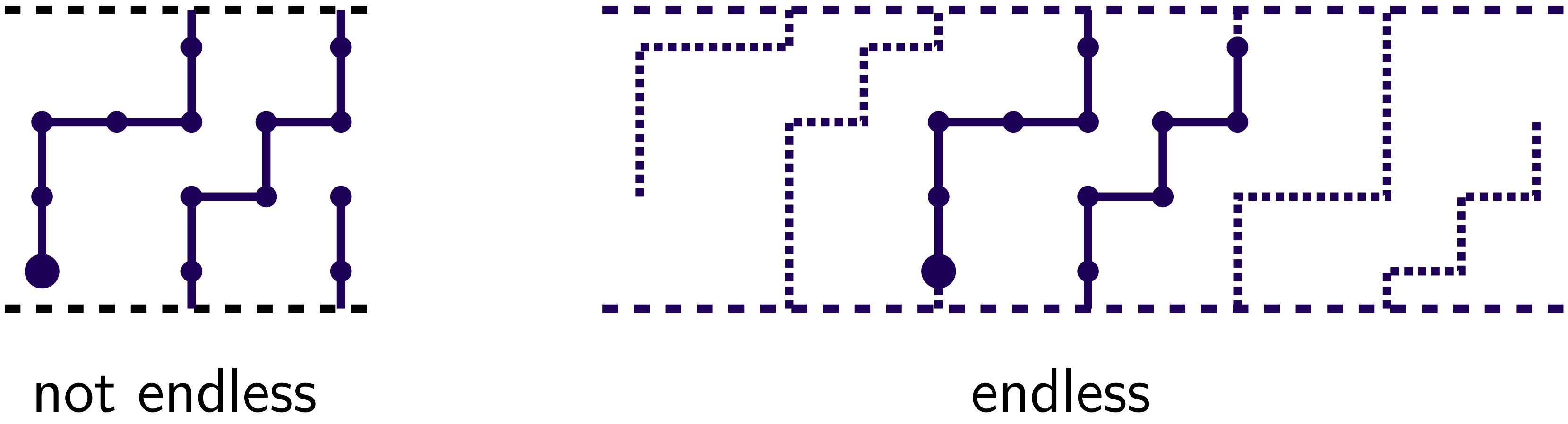
Directed walks on a cylinder



Directed walks which take north and east steps on a cylinder of height 4.

Endless condition restricts vertical steps at the start and end.

Directed walks on a cylinder



Directed walks which take north and east steps on a cylinder of height 4.

Endless condition restricts vertical steps at the start and end.

Directed walks on a cylinder

For a cylinder of height 2.

- SAW (Fibonacci numbers):

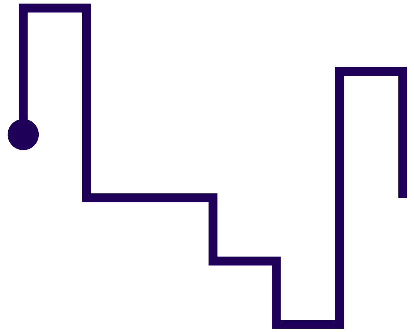
$$C(z) = \frac{1+z}{1-z-z^2} = 1 + 2z + 3z^2 + 5z^3 + 8z^4 + 13z^5 + \cdots$$

- Endless SAW (Lucas numbers):

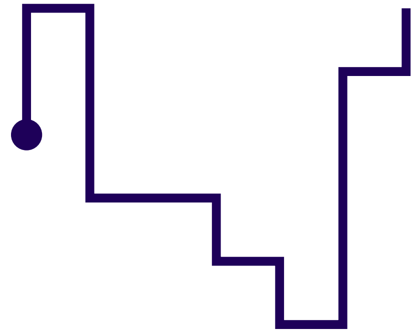
$$E(z) = \frac{z+2z^2}{1-z-z^2} = z + 3z^2 + 4z^3 + 7z^4 + 11z^5 + \cdots$$

$$e_n = \left(\frac{1}{2} + \frac{\sqrt{5}}{2}\right)^n + \left(\frac{1}{2} - \frac{\sqrt{5}}{2}\right)^n$$

Partially directed walks



not endless



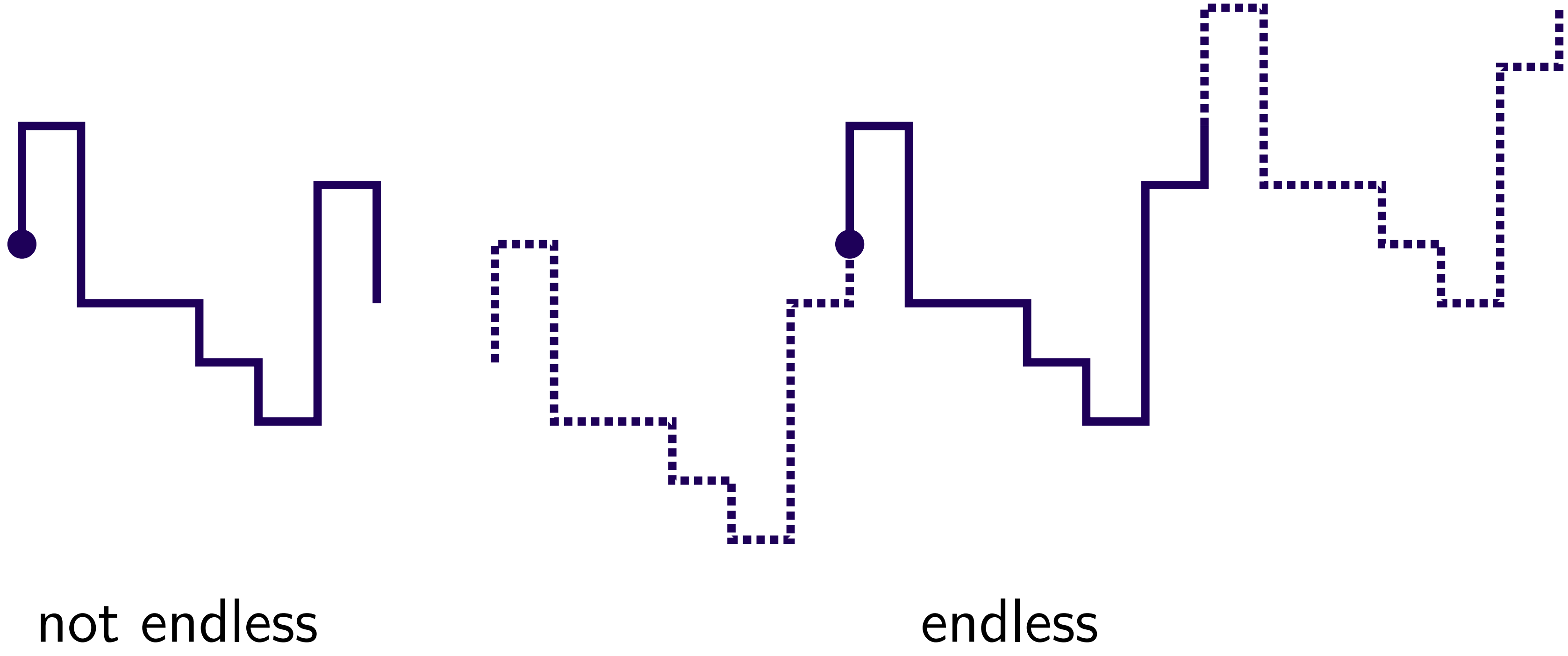
endless

$$C(z) = \frac{1+z}{1-2z-z^2}$$

$$E(z) = \frac{3z-2z^2-3z^3}{1-3z+z^2+z^3}$$

$$e_n = 1 + (1-\sqrt{2})^n + (1+\sqrt{2})^n$$

Partially directed walks



$$C(z) = \frac{1+z}{1-2z-z^2}$$

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$$e_n = 1 + (1-\sqrt{2})^n + (1+\sqrt{2})^n$$

How to study eSAWs?

Model is at least as difficult to solve as SAW.

So, we use numerical approaches:

- Enumeration (hard to see how to use transfer matrix method efficiently)
- **Monte Carlo sampling**

The best Monte Carlo algorithm for SAW is the pivot algorithm.

Pivot algorithm

Procedure:

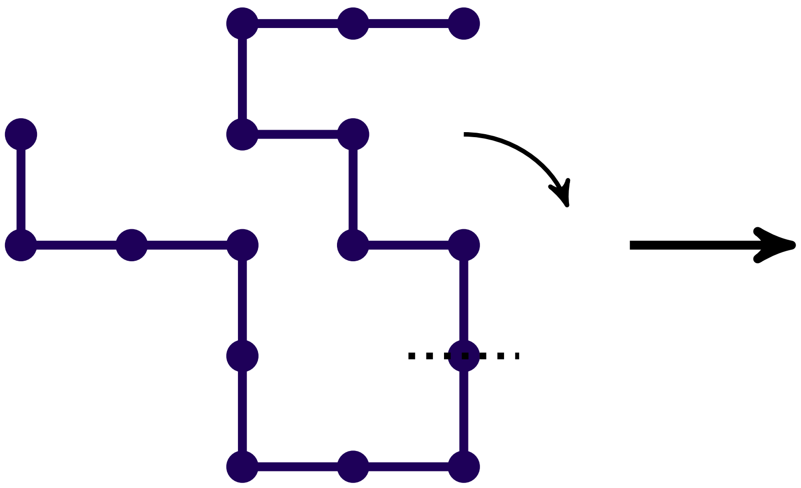
- Choose a pivot site at random.
- Then rotate or reflect one of the two parts of the walk.
- Retain new walk if it is self-avoiding, otherwise restore original walk.

Large change in observables such as size with each successful pivot.

Ergodic, samples SAWs uniformly at random.

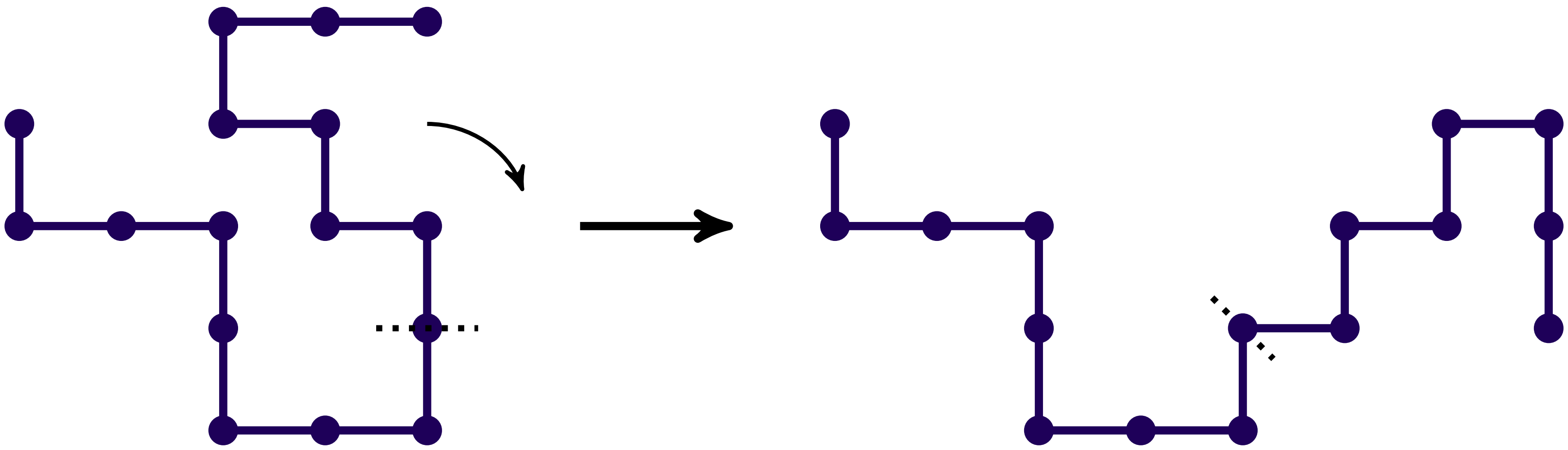
Binary tree data structure provides a very efficient implementation.

Pivot algorithm



Example pivot move

Pivot algorithm



Example pivot move

Pivot algorithm for eSAWs

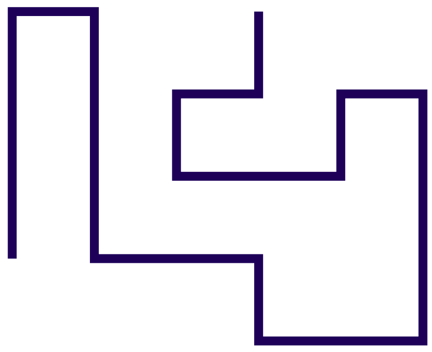
Procedure:

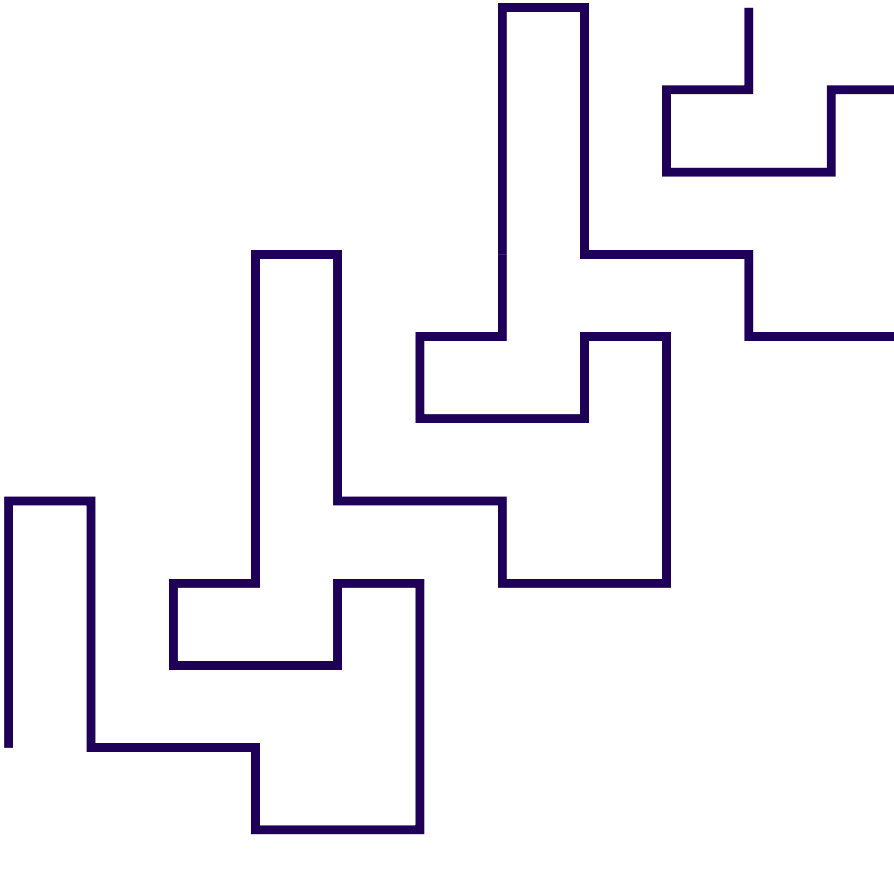
- Choose arbitrary start point for eSAW.
- Choose arbitrary pivot site.
- Rotate or reflect from the pivot site to the end, while leaving other piece unchanged.
- Test if resulting endless walk is self-avoiding.

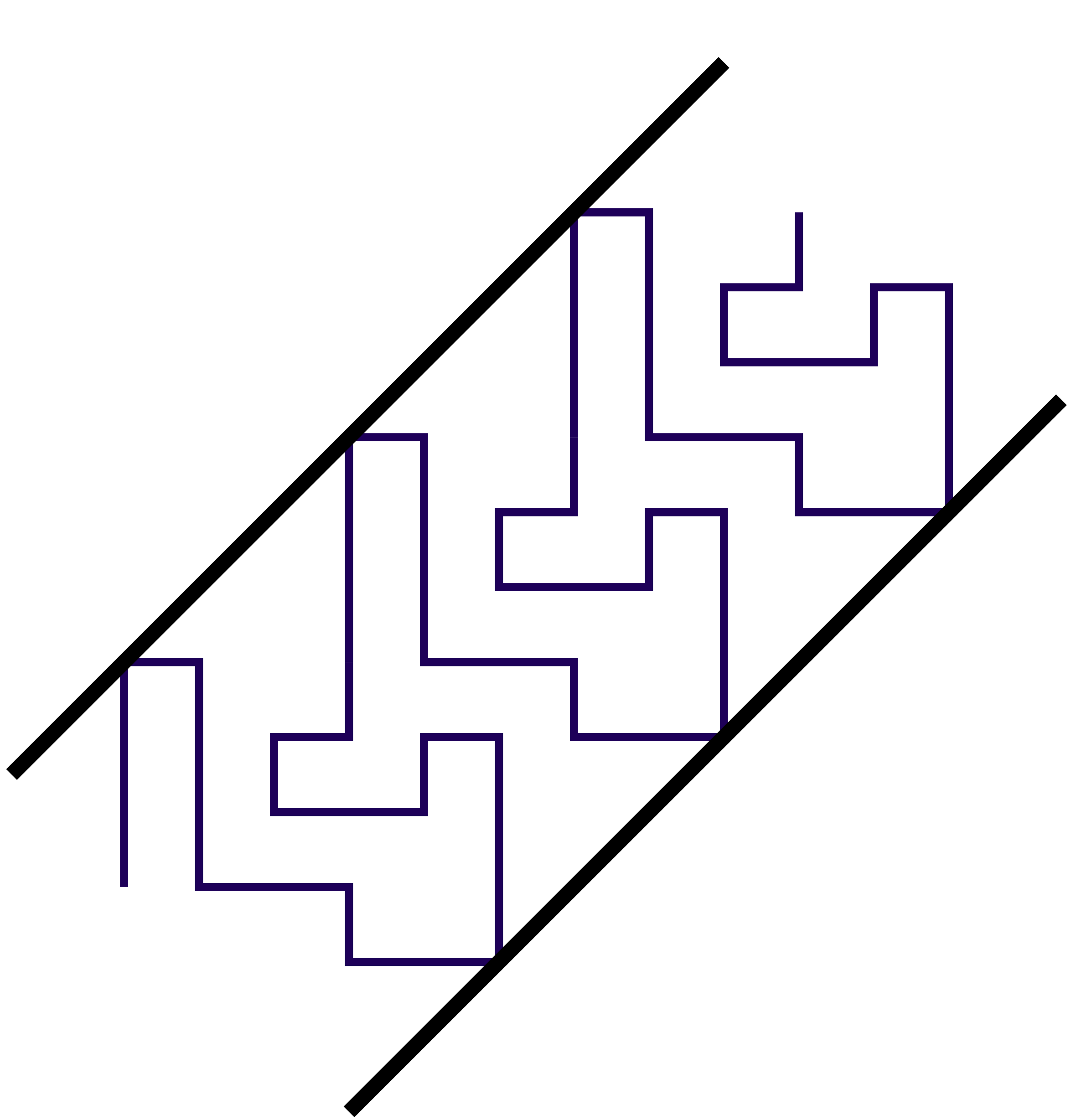
Note: there are effectively *two* pivot sites for the eSAW pivot move. This reduces the probability of it being successful.

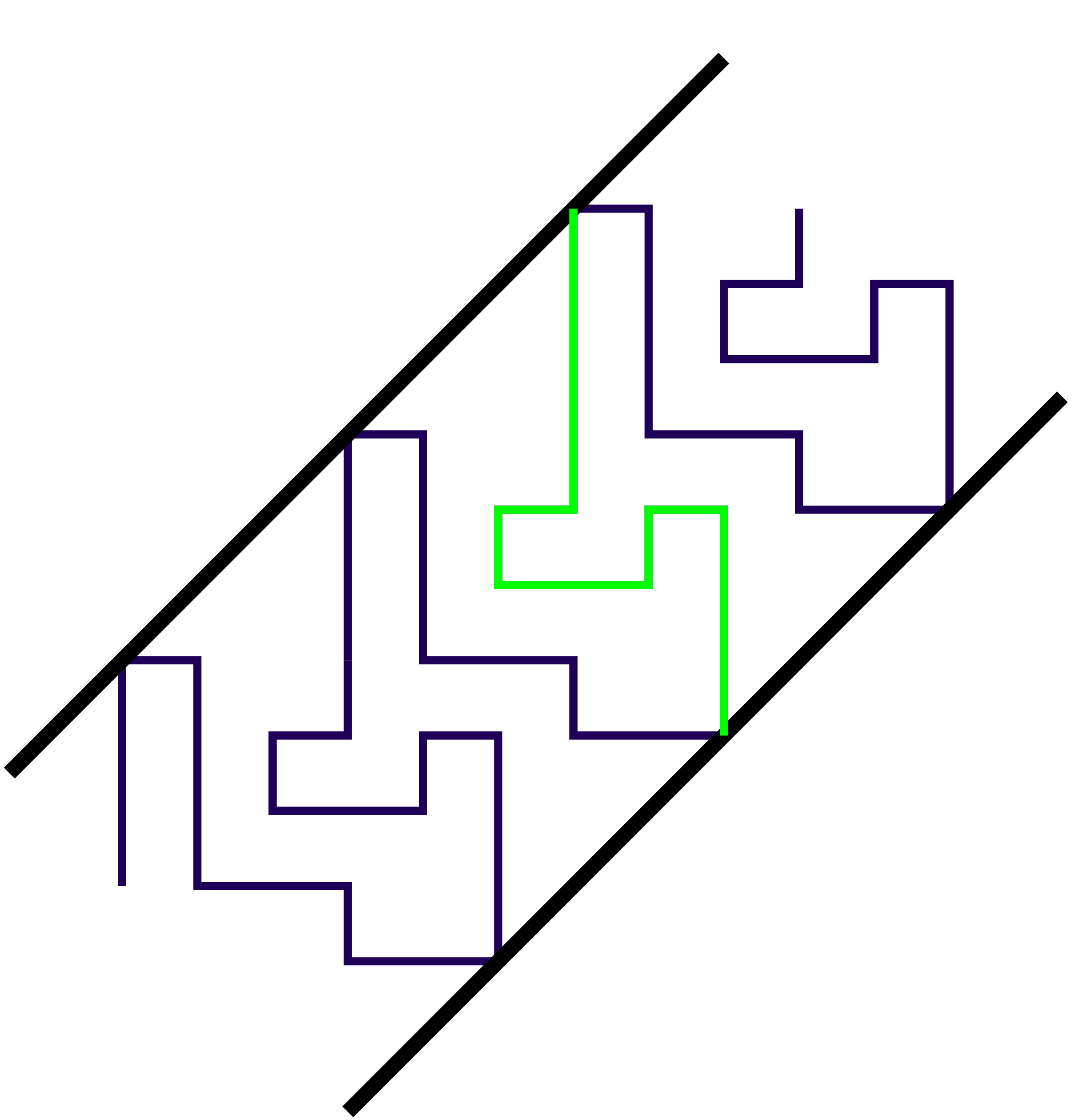
Possible to prove that it is ergodic.

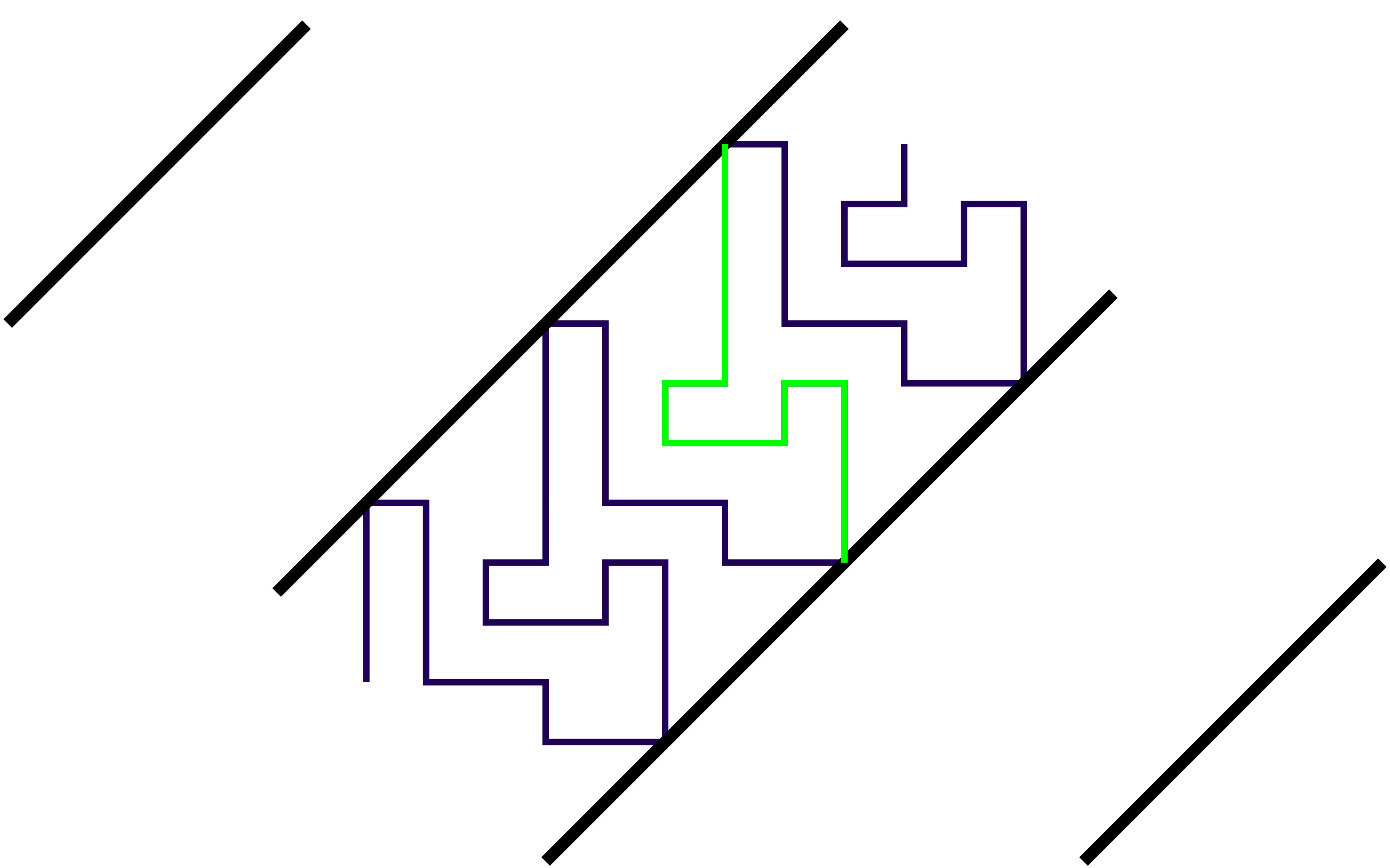
Here follows an example pivot move.

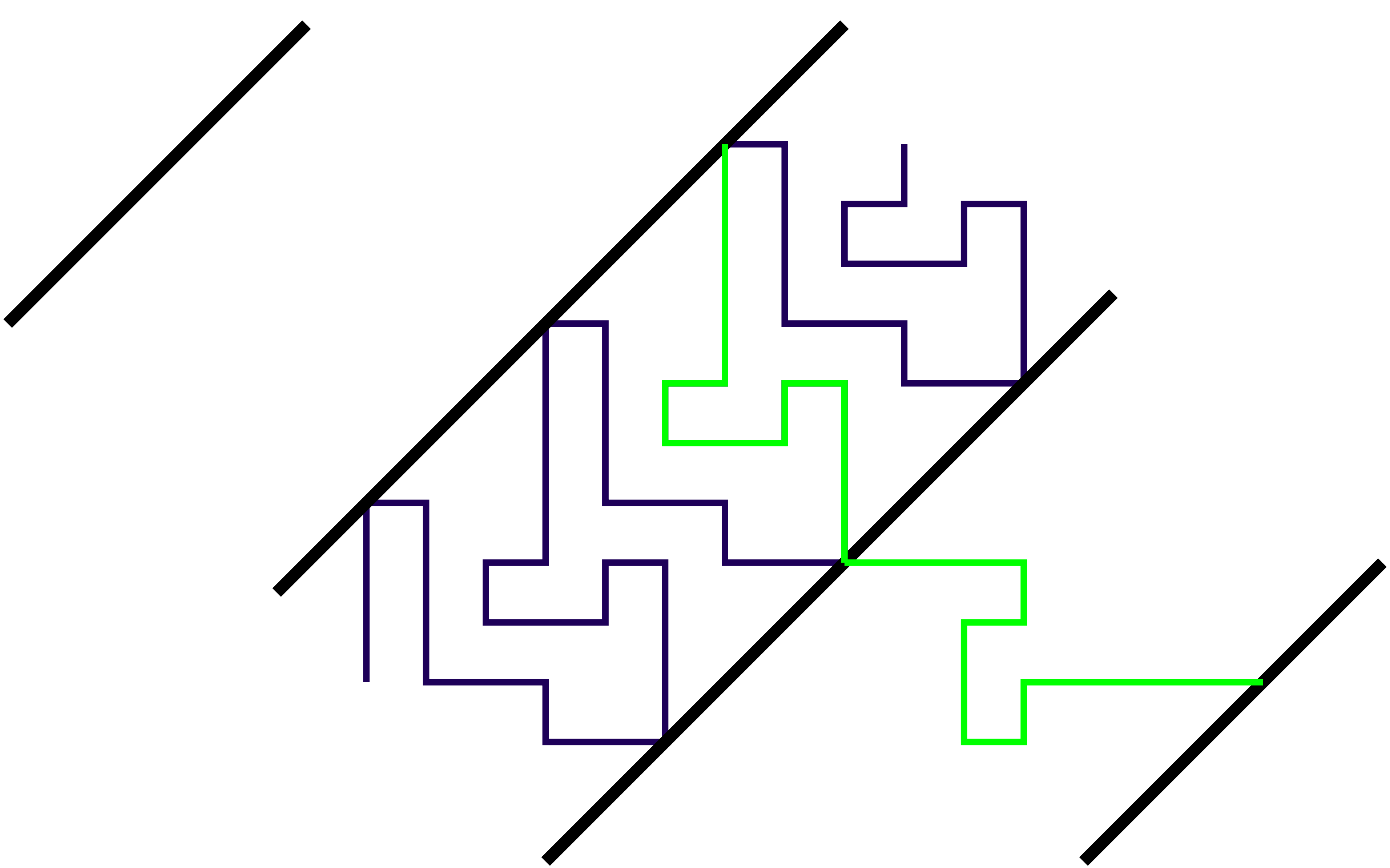


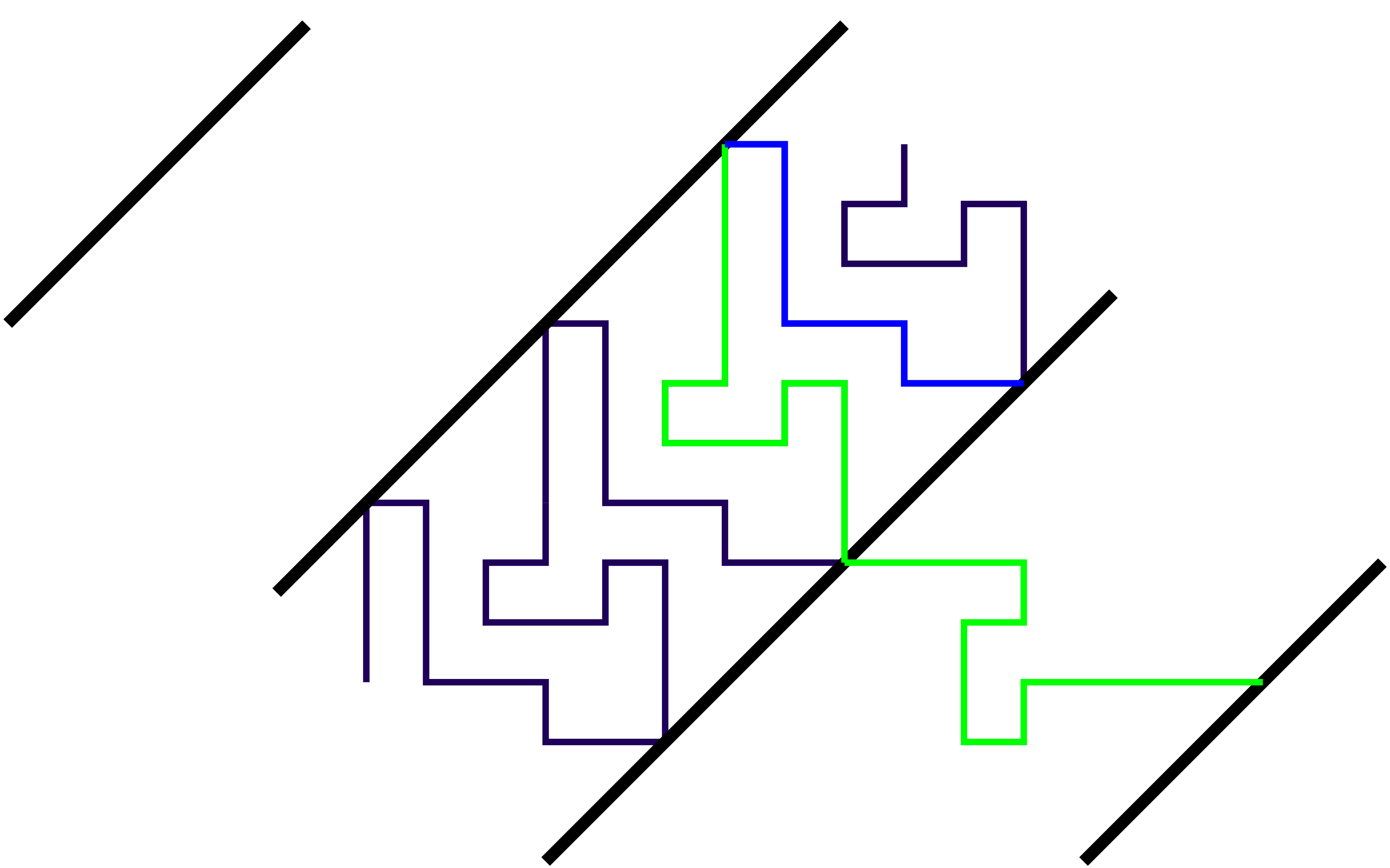


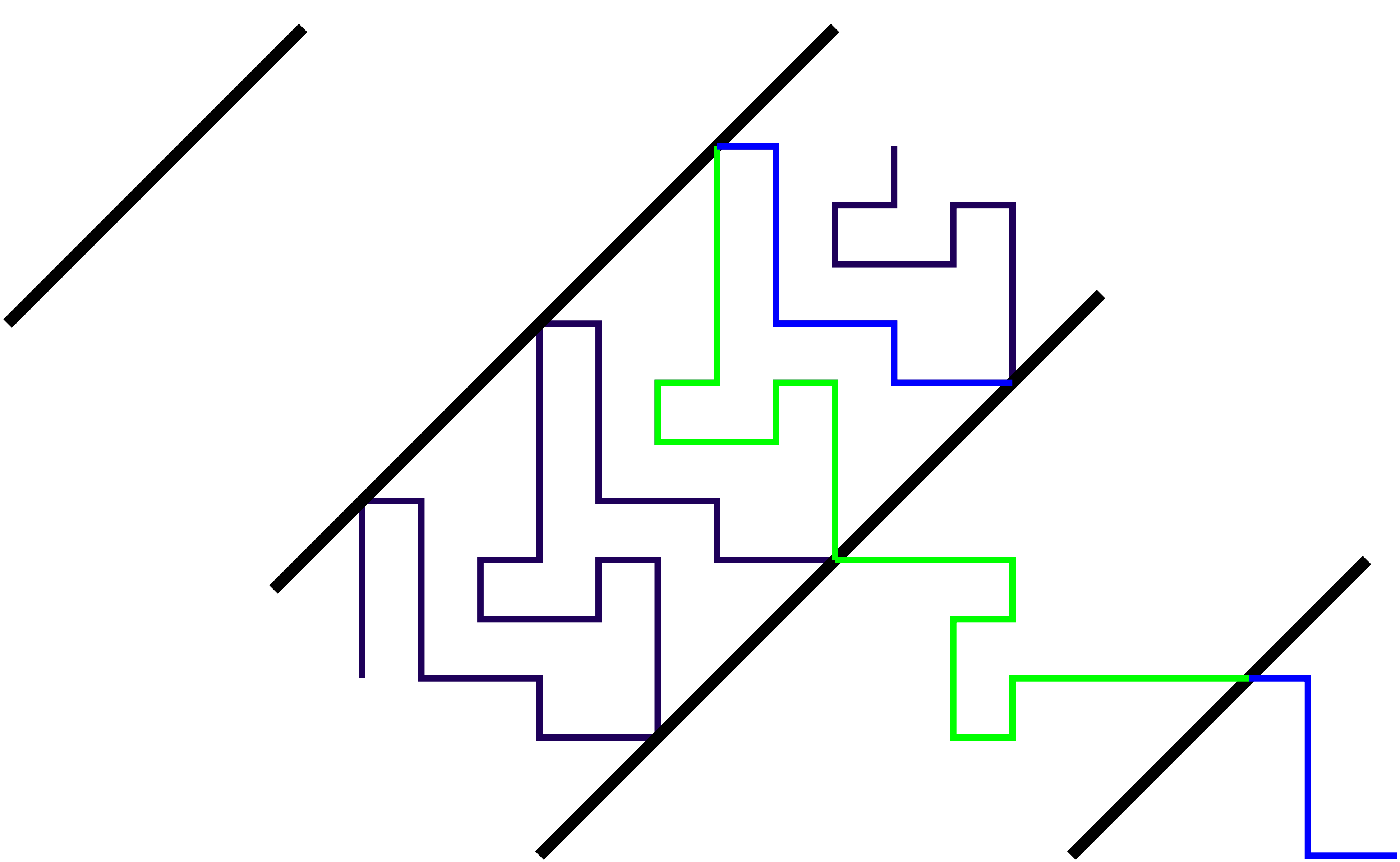


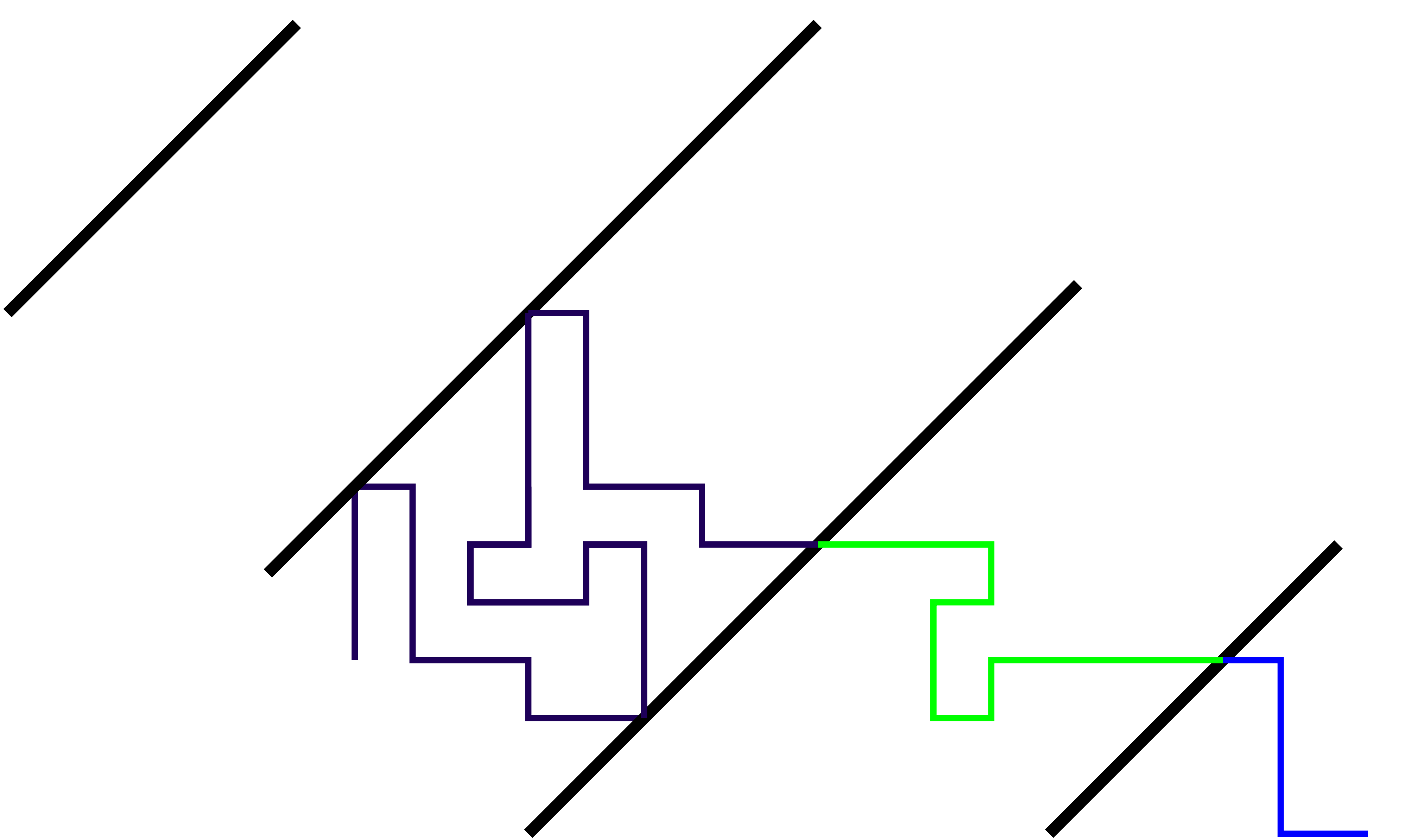


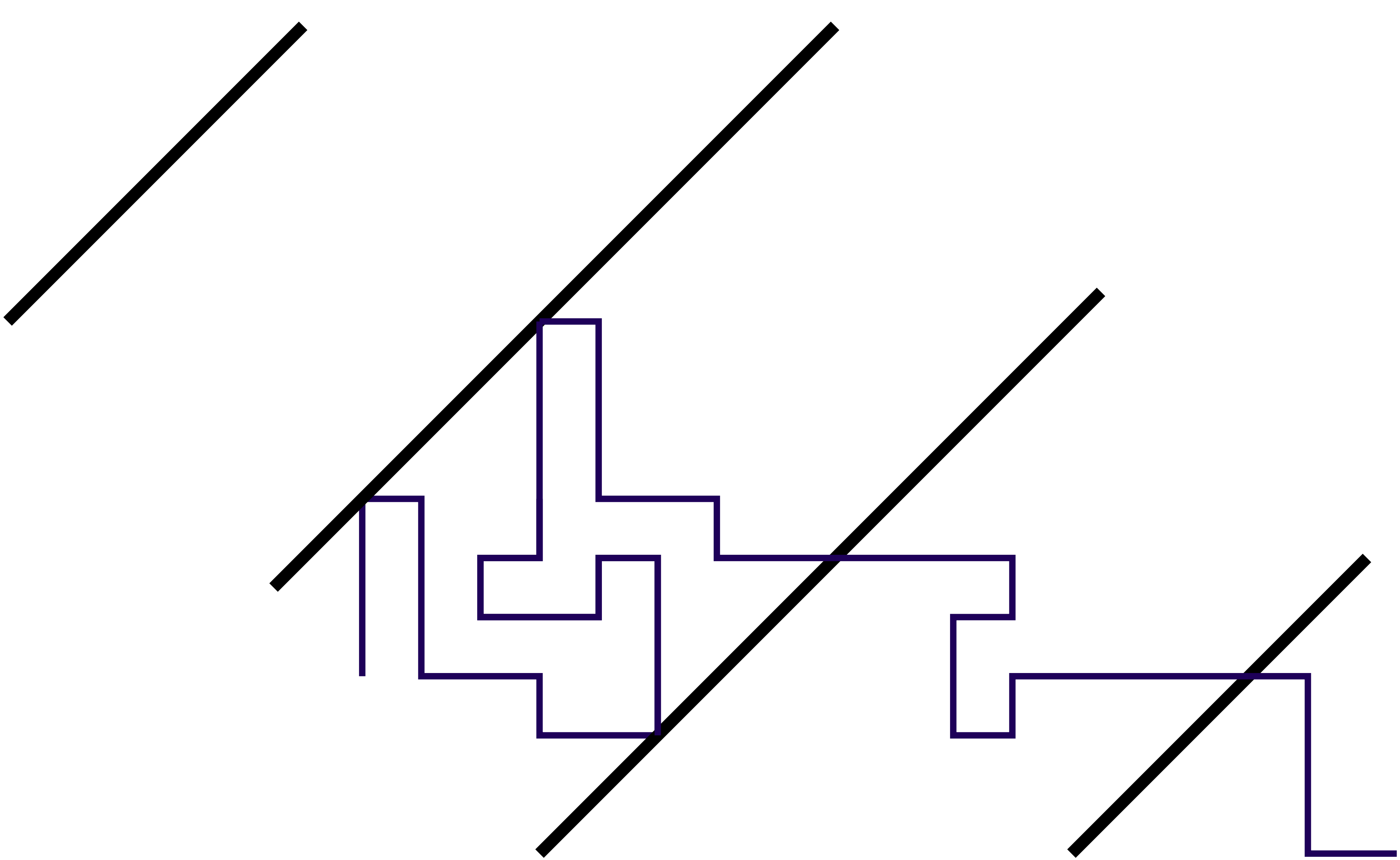


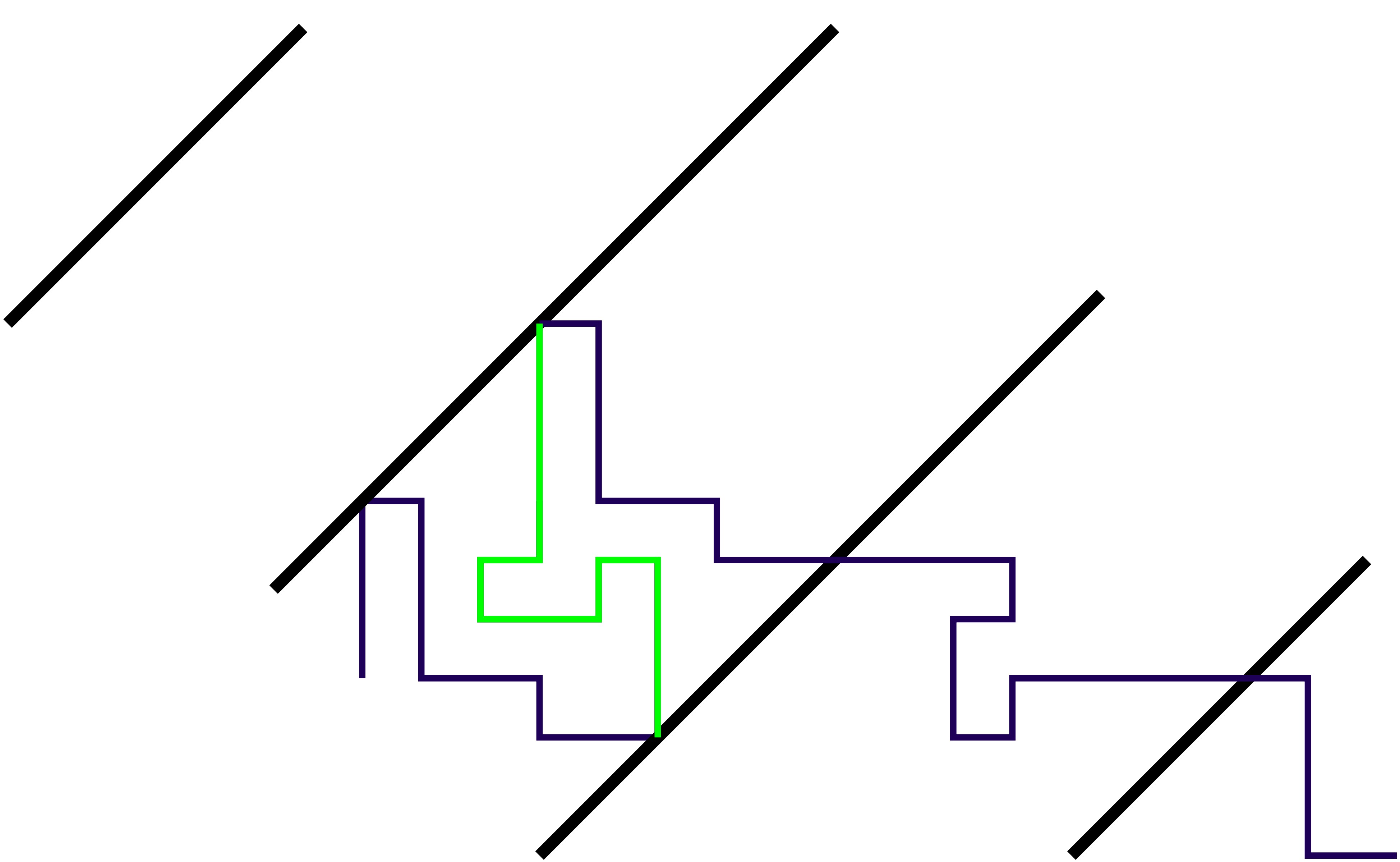


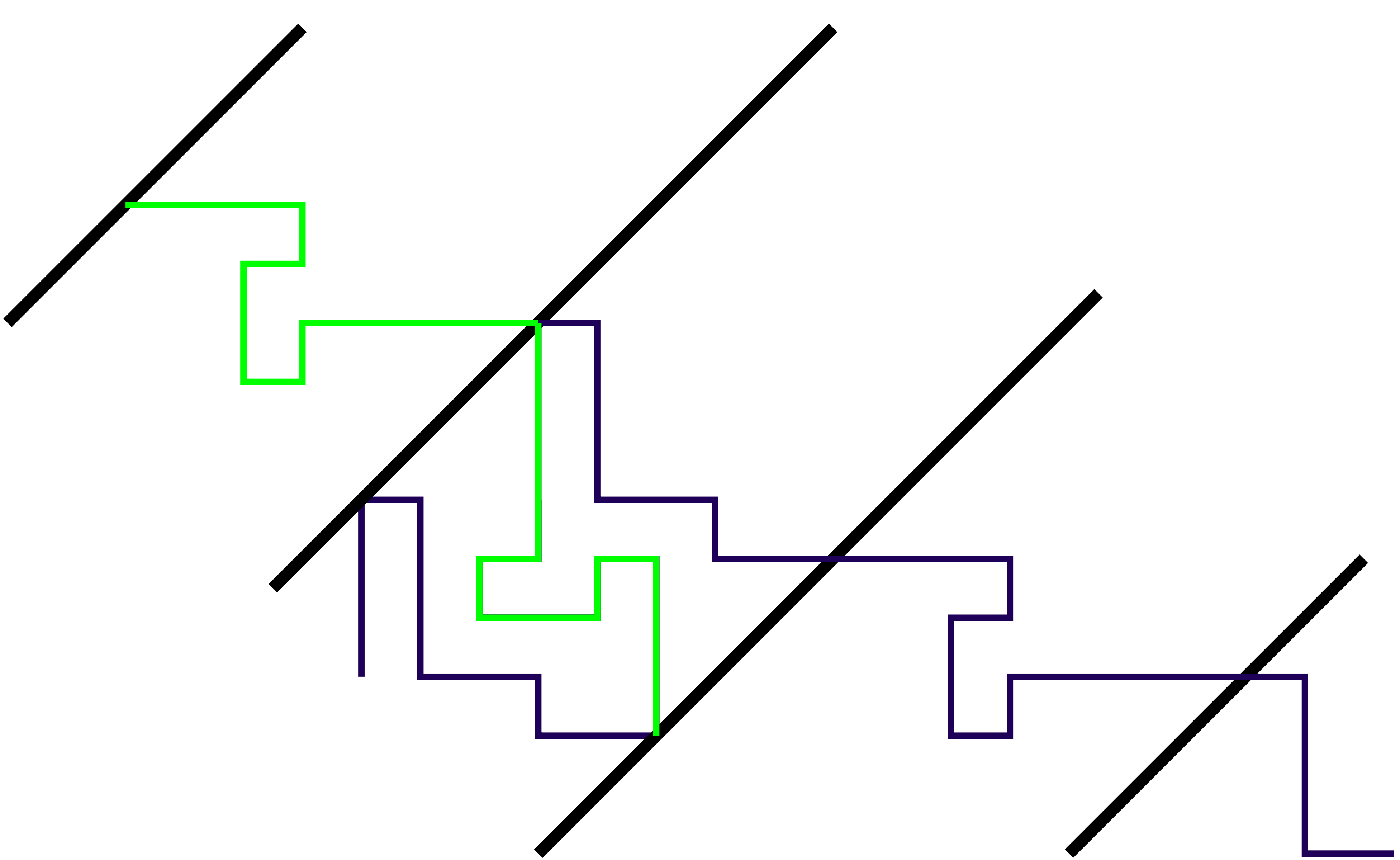


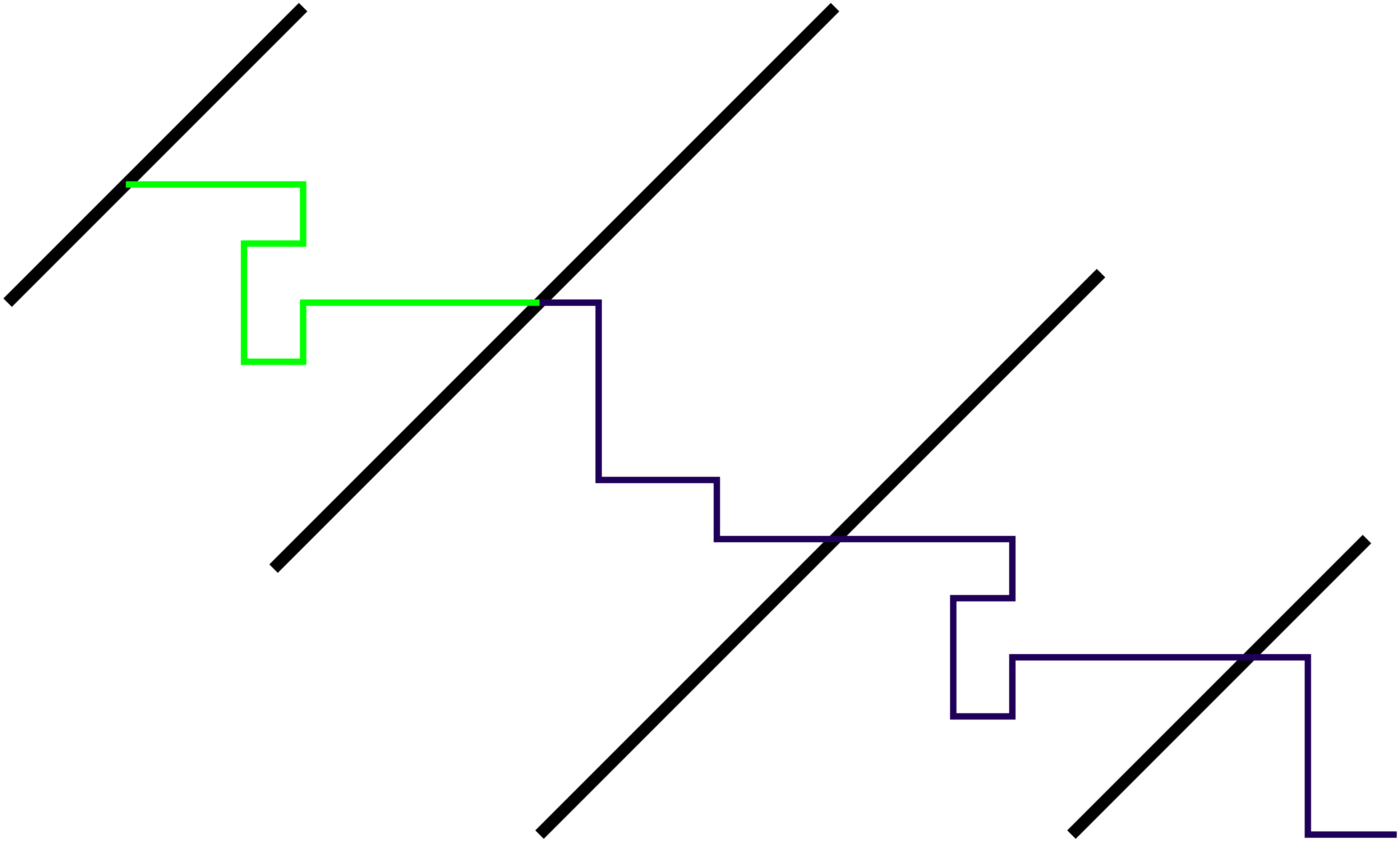


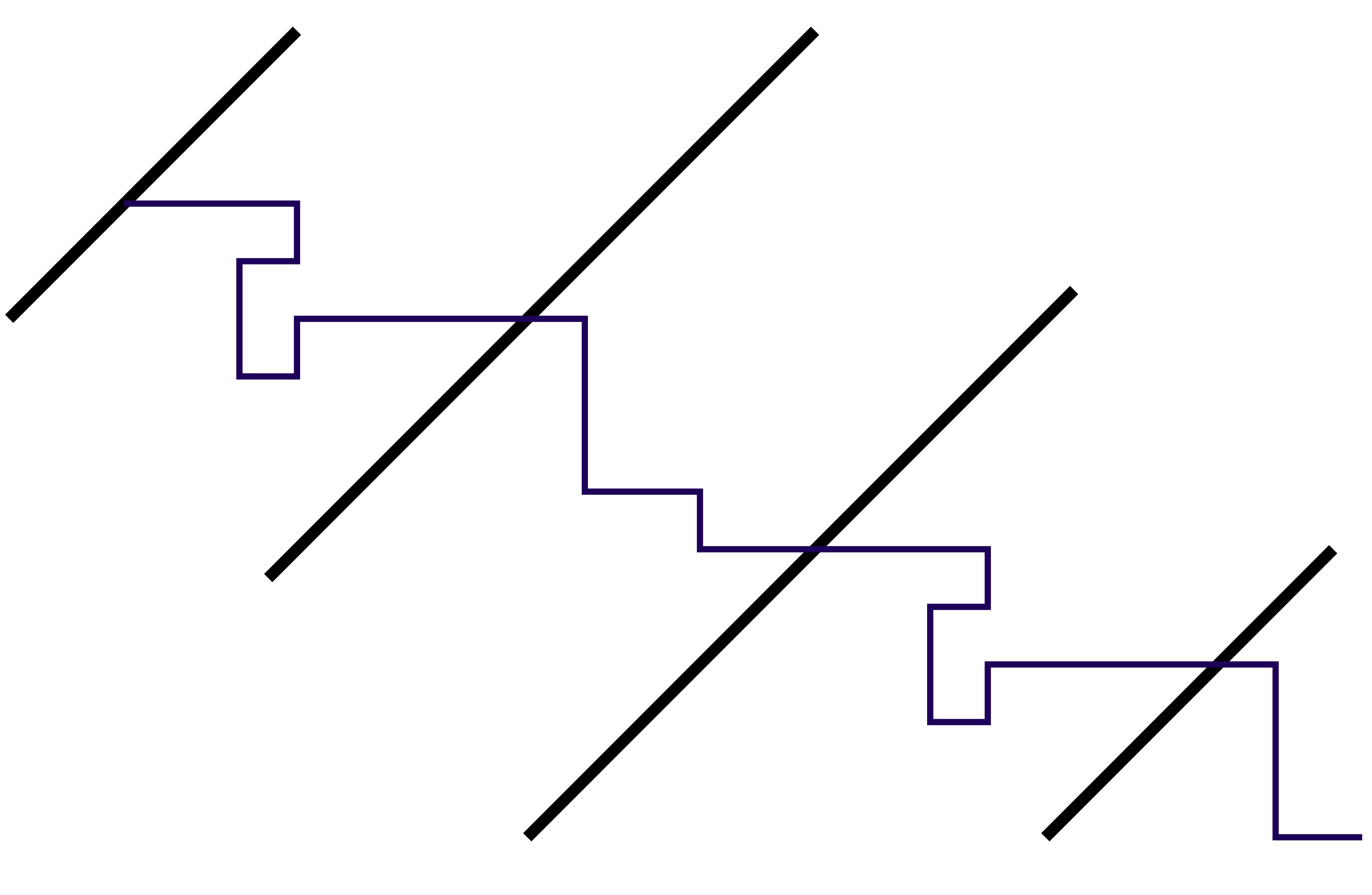


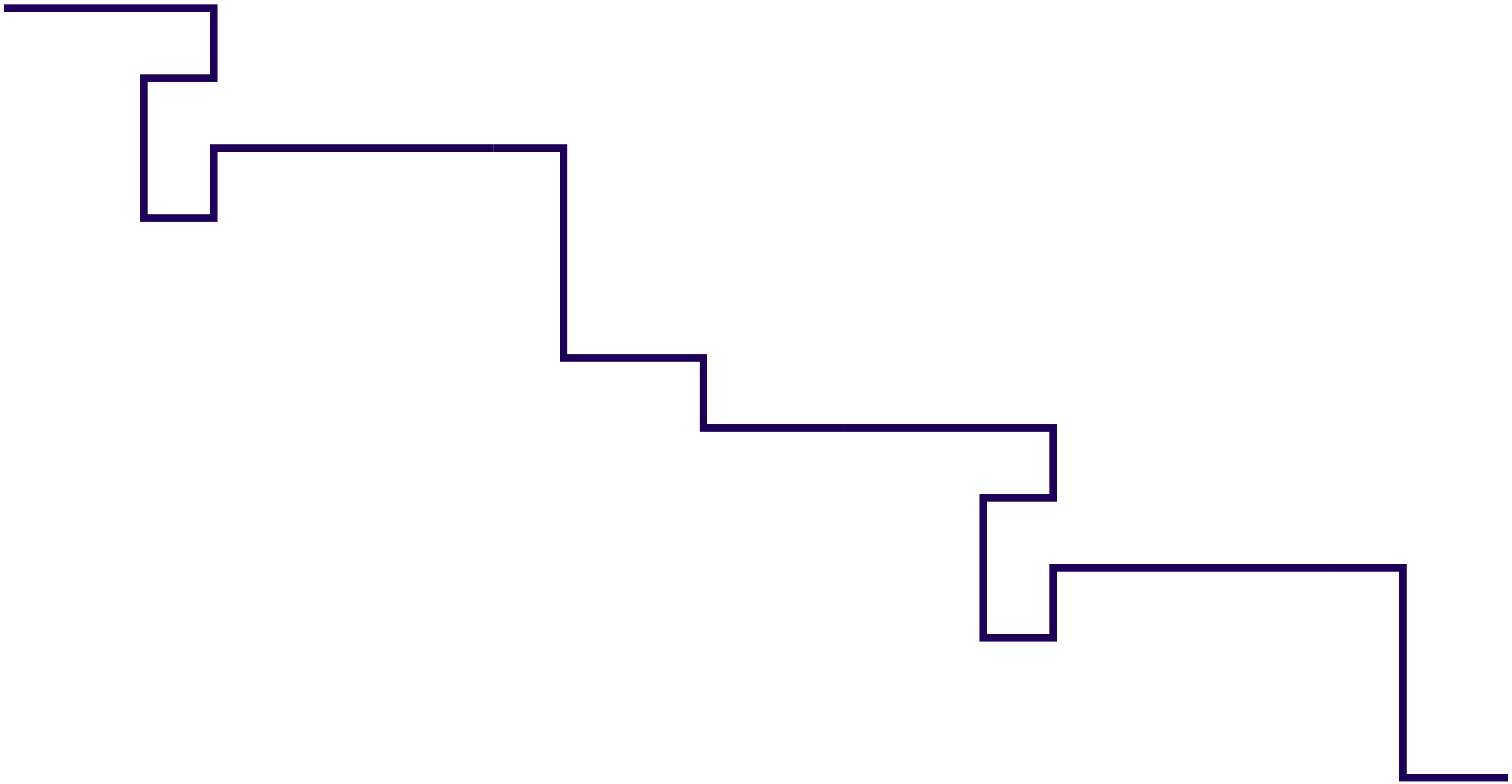












Bridges

N-step walk of N steps has $N+1$ sites: 0, 1, . . ., N.

Bridges are SAWs which satisfy $y(0) < y(i) \leq y(N)$.

There is a "break edge" at the start of the walk. (Can draw a line or plane through it and cut no other edges.)

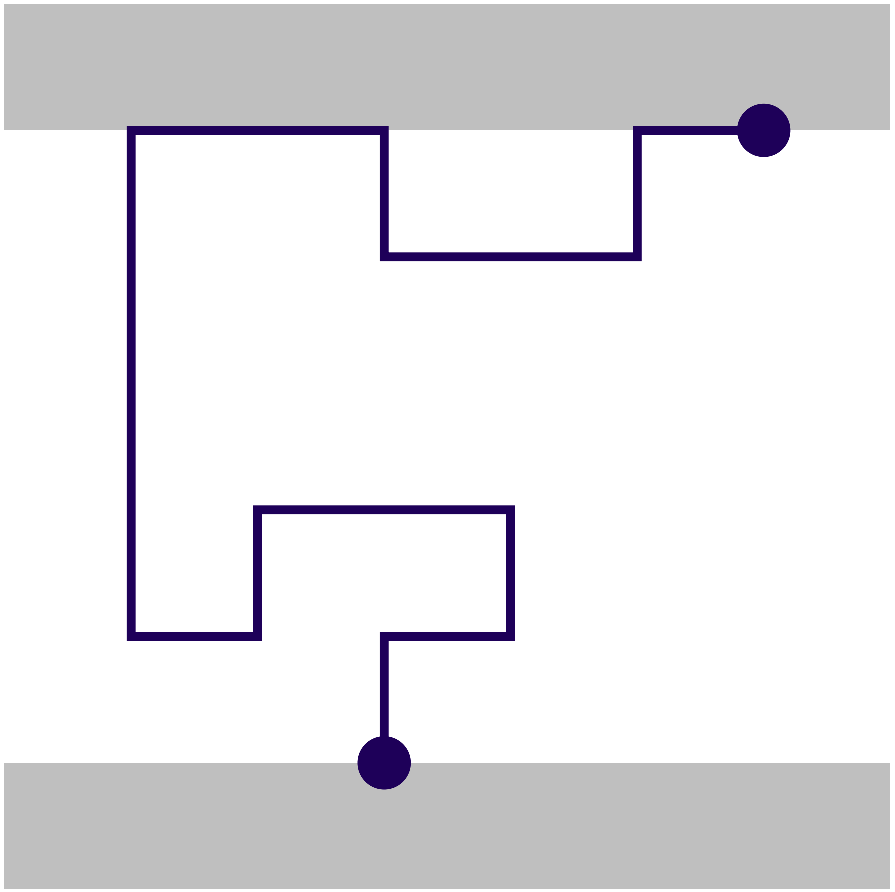
Bridges can be concatenated and are guaranteed to remain self-avoiding.

In particular, a bridge can be concatenated with itself.

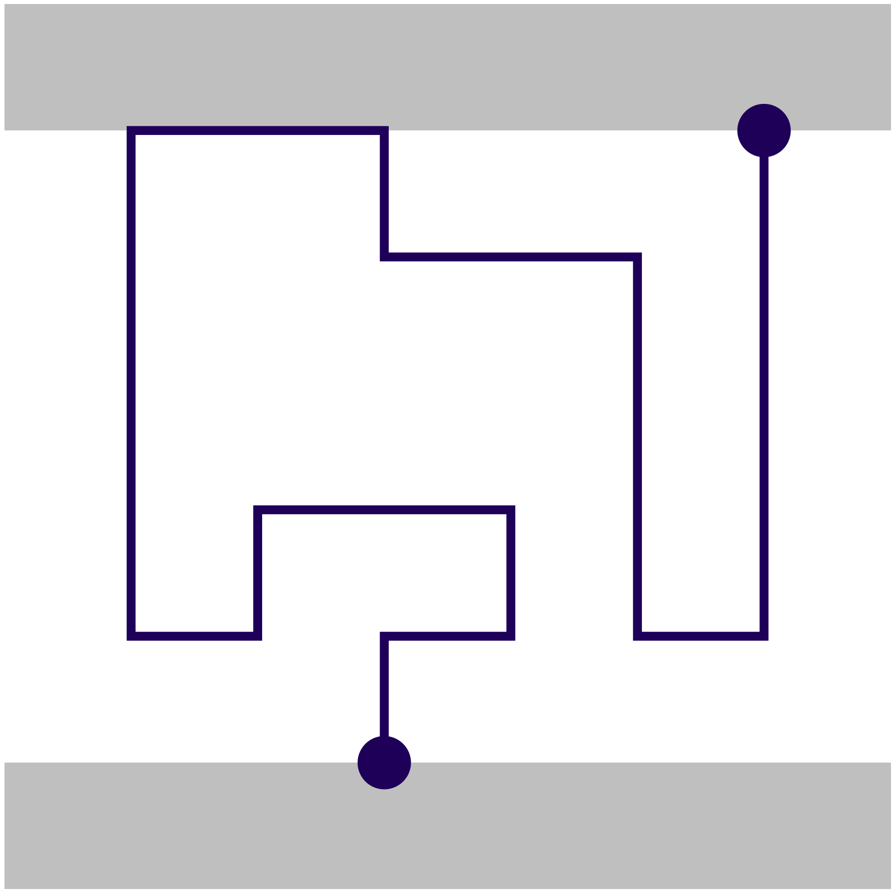
Thus bridges are a subset of eSAWs.

An irreducible bridge is a bridge with exactly one break edge.

Bridges



Bridge



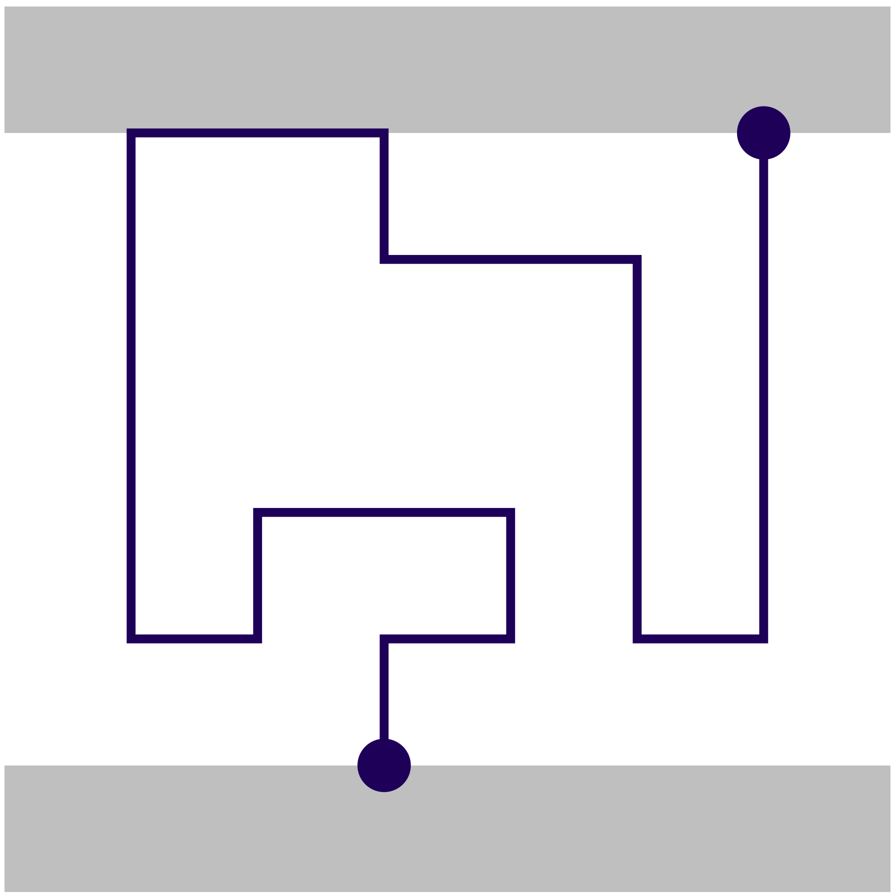
Irreducible bridge

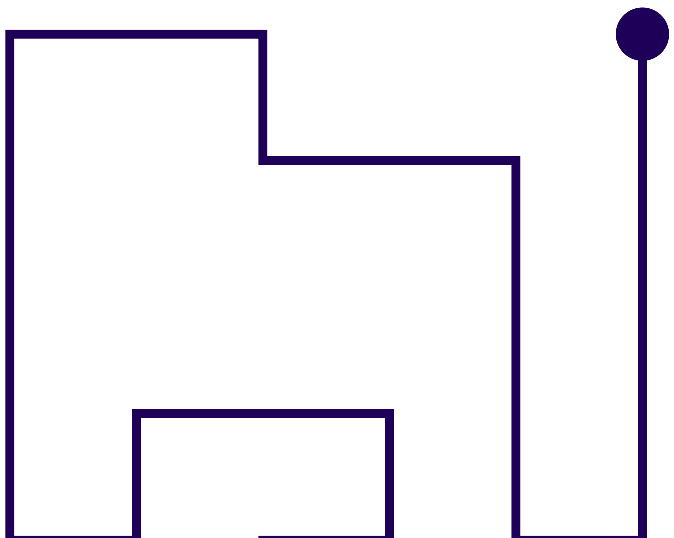
Bridges

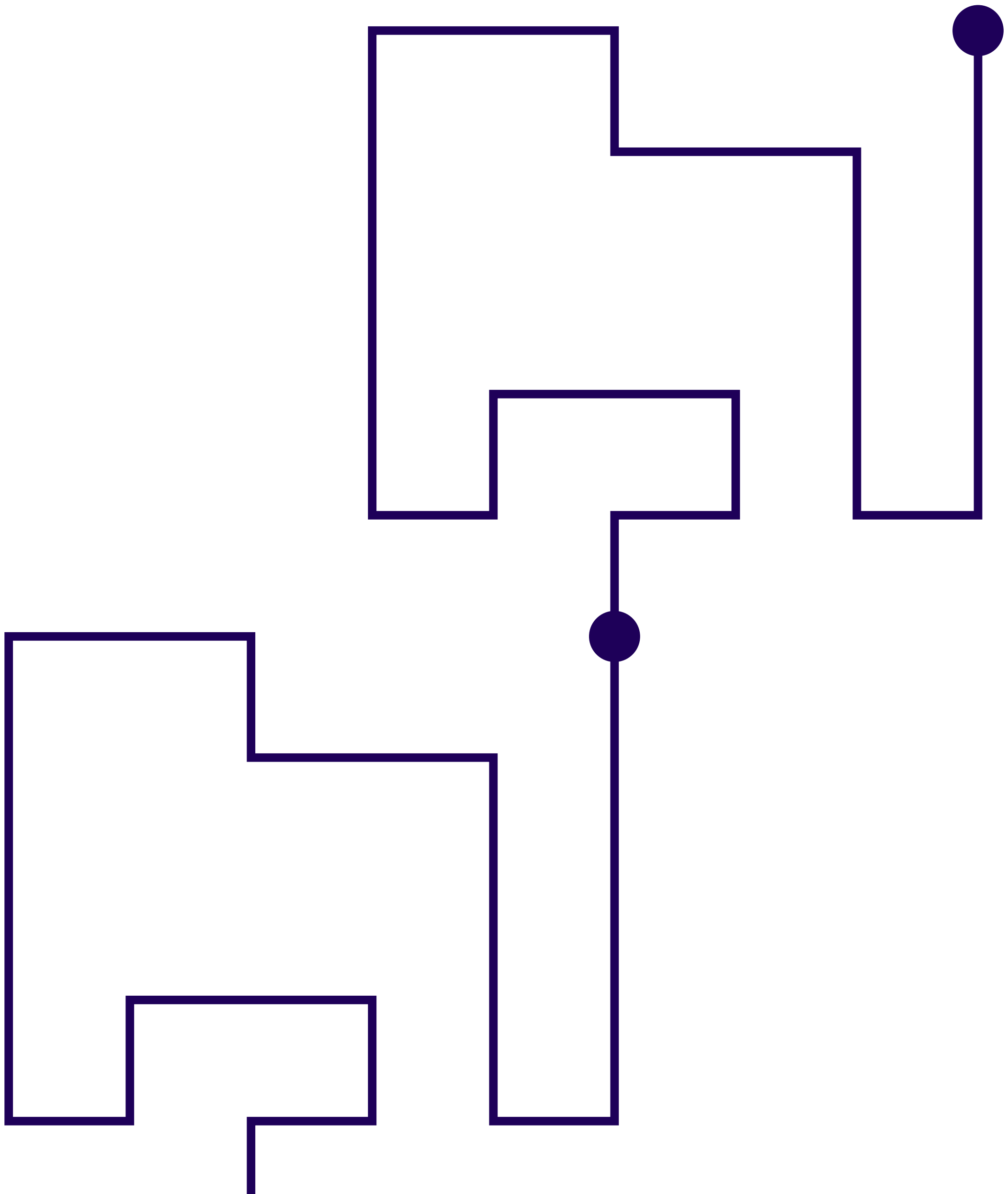
Let's go one step further: what if we consider endless SAWs with break edges, but no longer care if the first edge is a break edge?

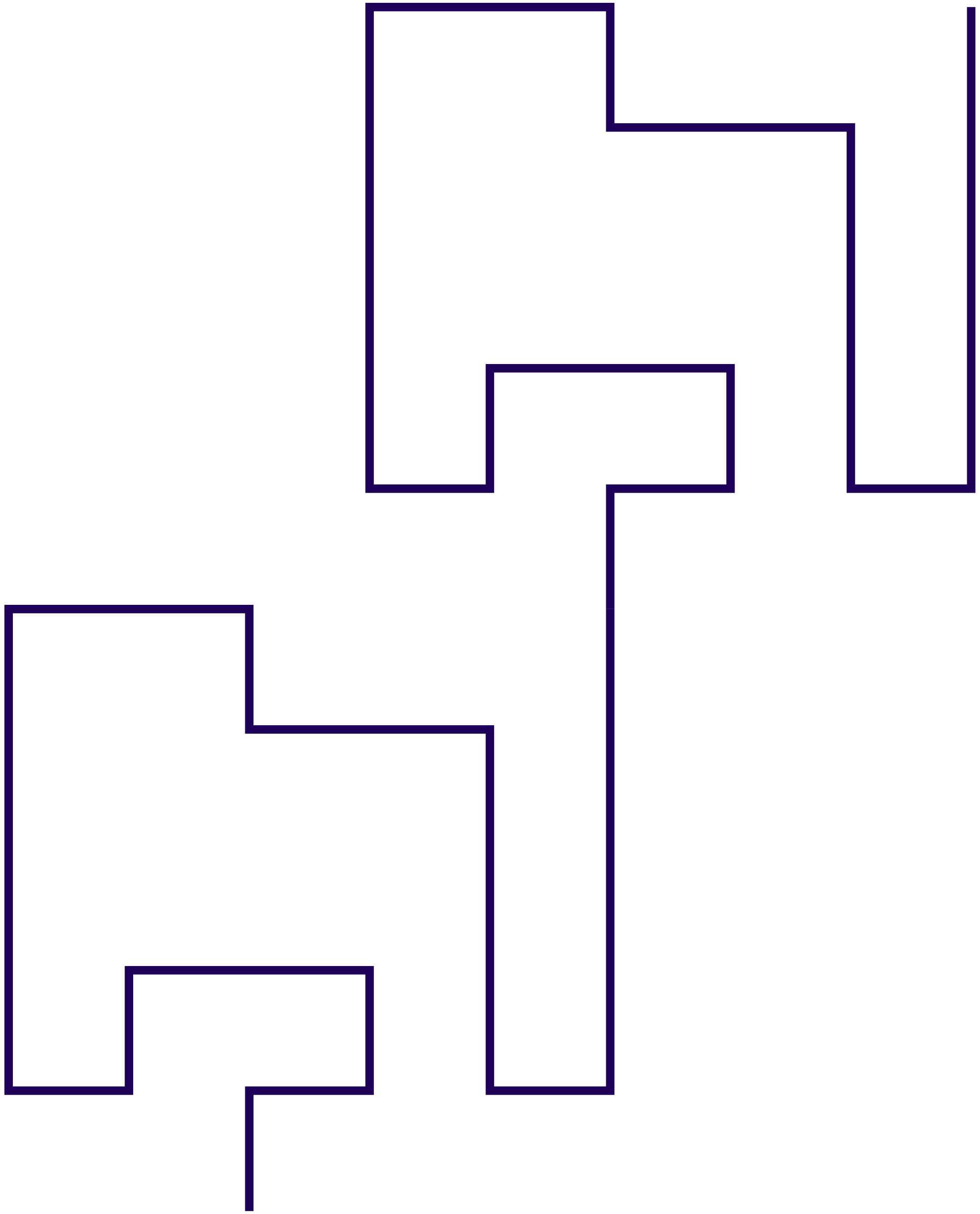
These are "endless bridges".

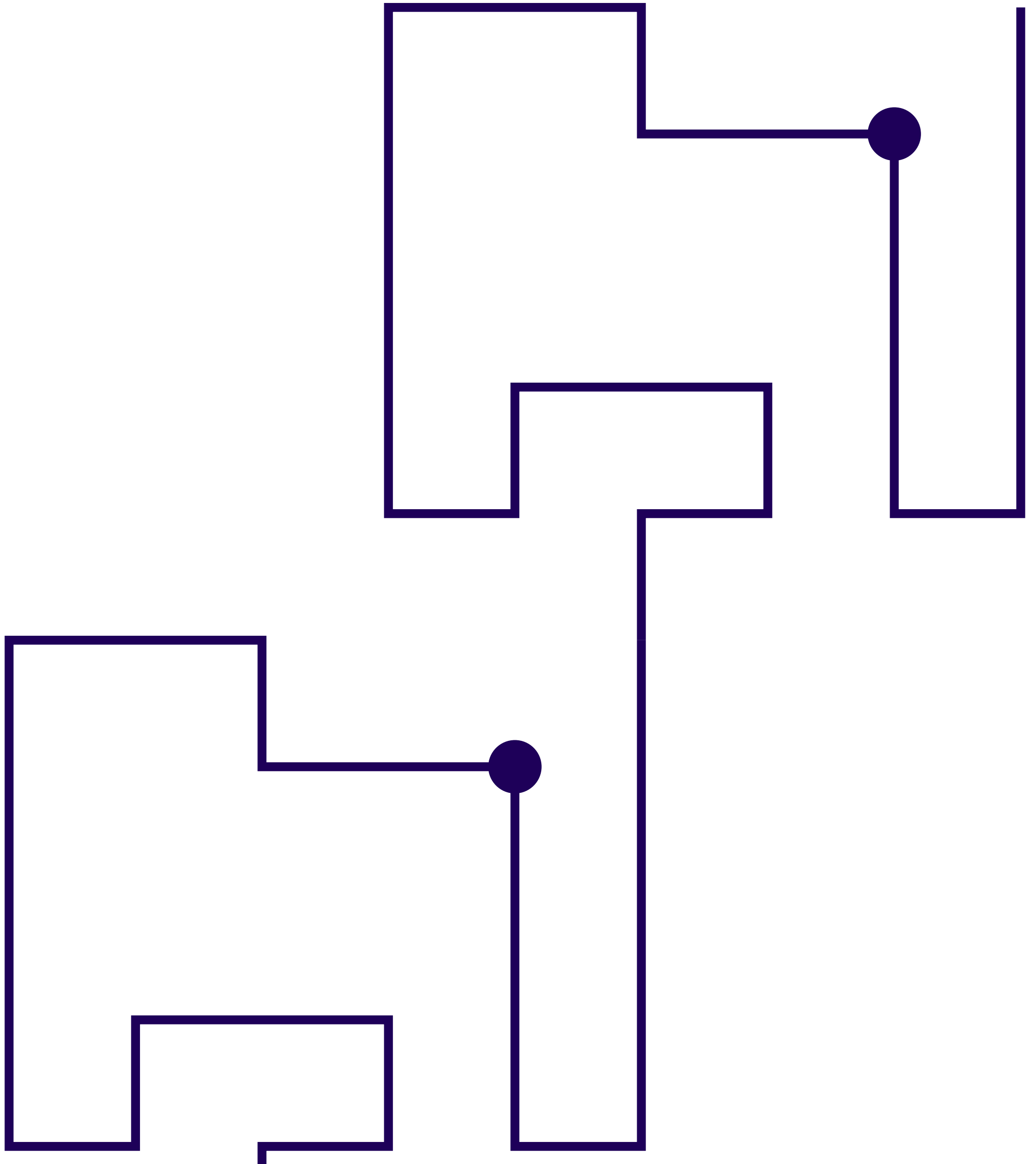
Endless bridges are also a subset of eSAWs.

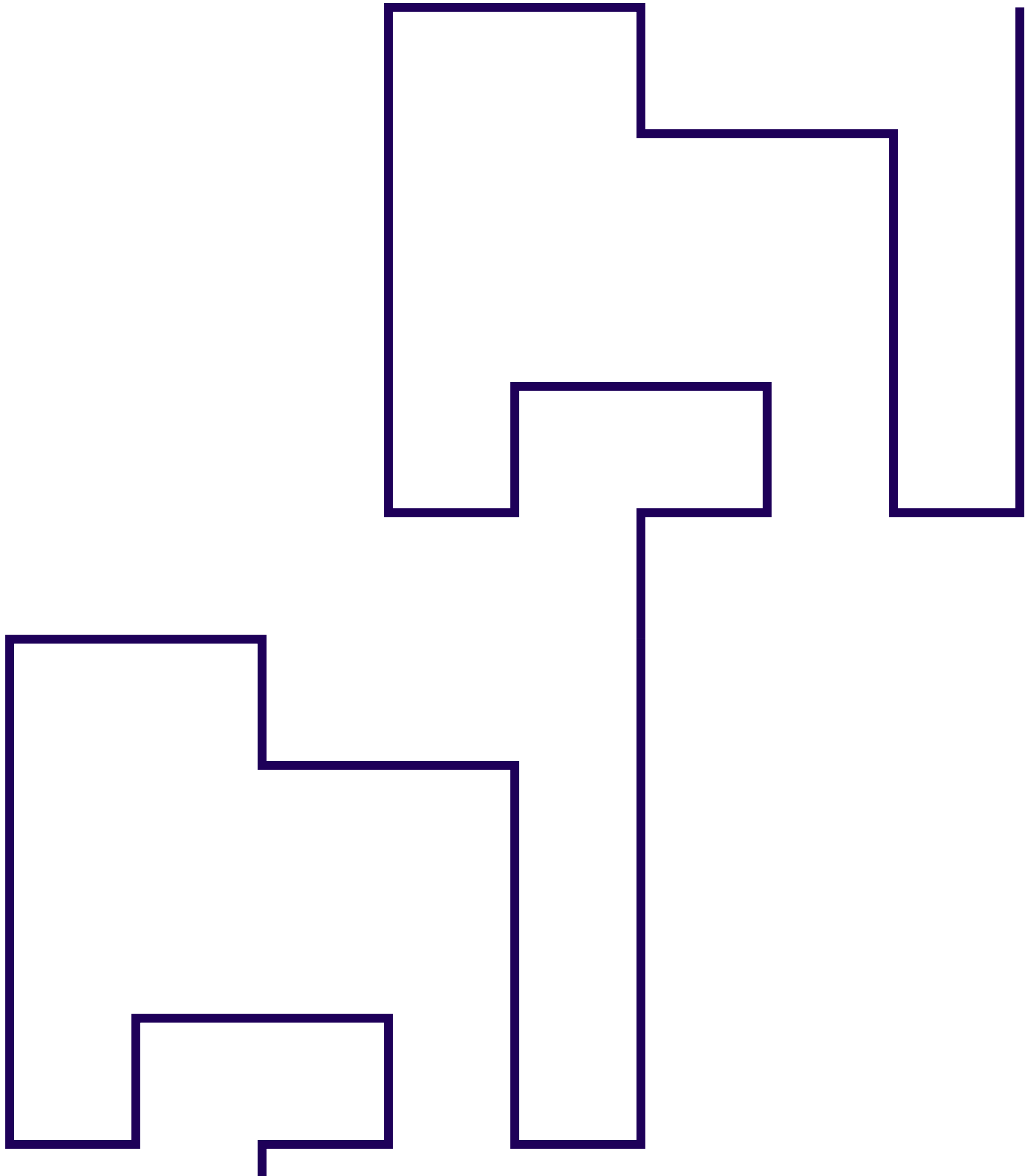


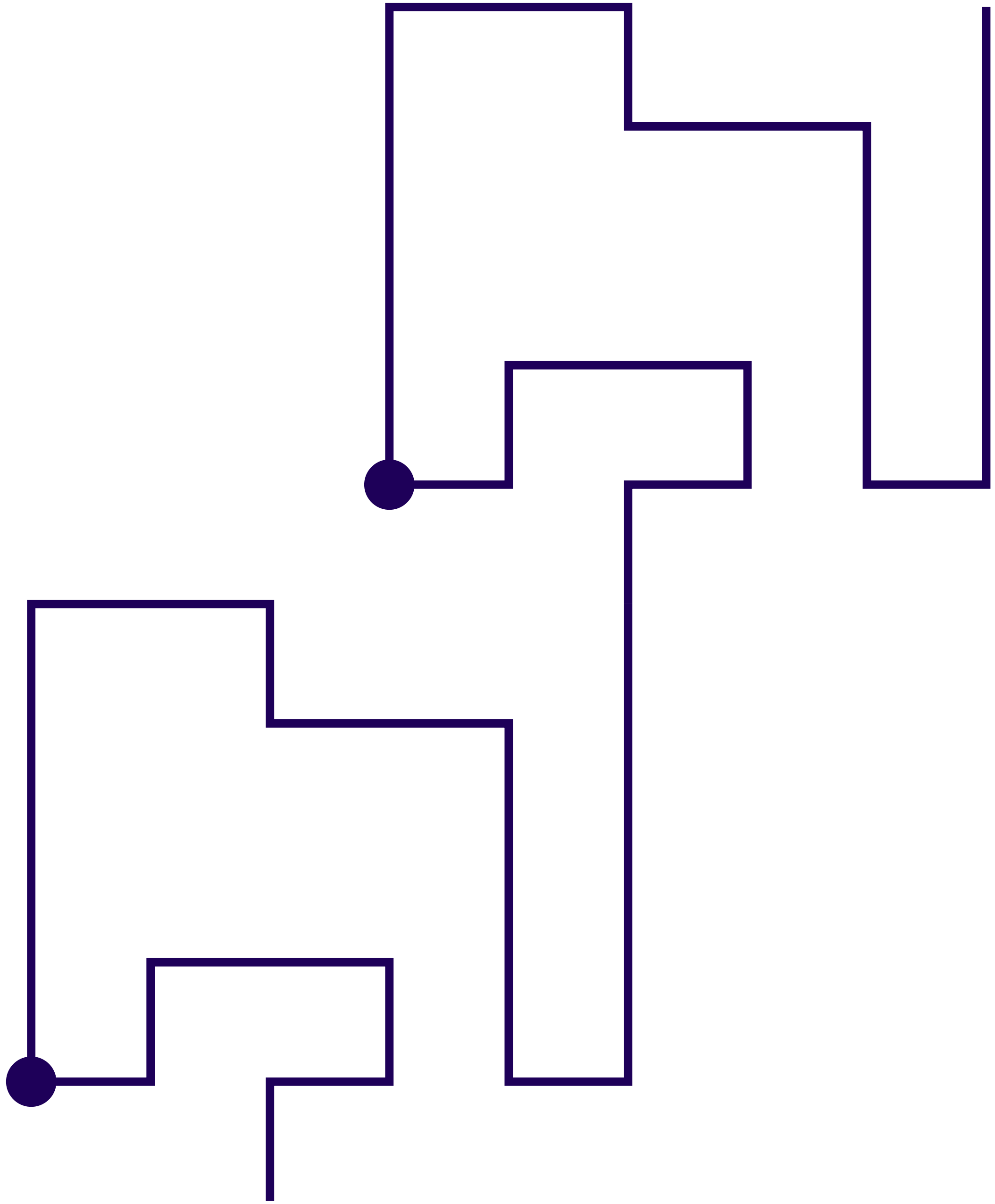


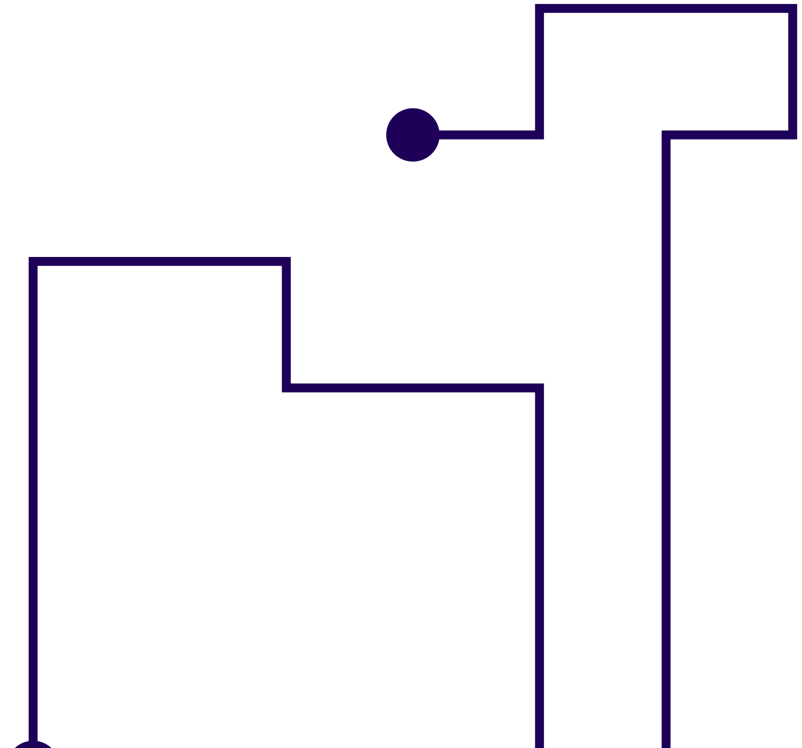












Bridges

Let $B(z)$ be the generating function of bridges. (Set $b_0 = 1$.)

Let $I(z)$ be the generating function of irreducible bridges.

Each irreducible bridge of n steps has n associated endless irreducible bridges.

$$
\begin{aligned}
ei_n &= n\, i_n \\
EI(z) &= \sum_{n=1}^{\infty} ei_n z^n = \sum_{n=1}^{\infty} n\, i_n z^n \\
&= \sum_{n=1}^{\infty} i_n z (z^n)' \\
&= z \left(\sum_{n=1}^{\infty} i_n z^n \right)' \\
&= z I'(z)
\end{aligned}
$$

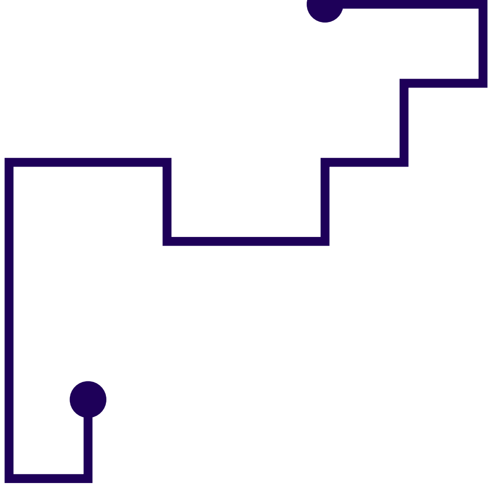
Bridges

Every bridge is either empty, or an irreducible bridge followed by a bridge.

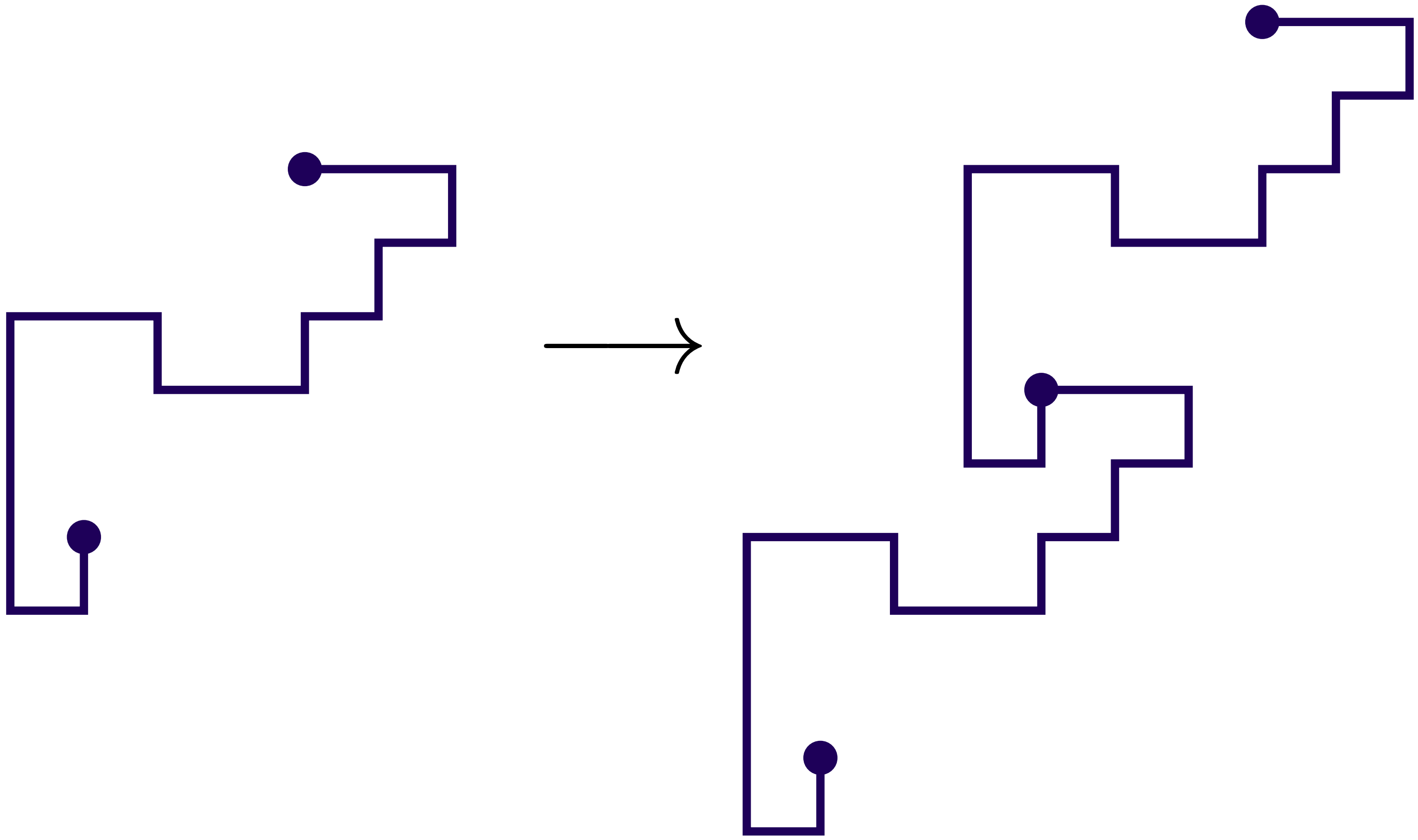
$$B(z) = 1 + I(z)B(z)$$

$$B(z) = \frac{1}{1 - I(z)}$$

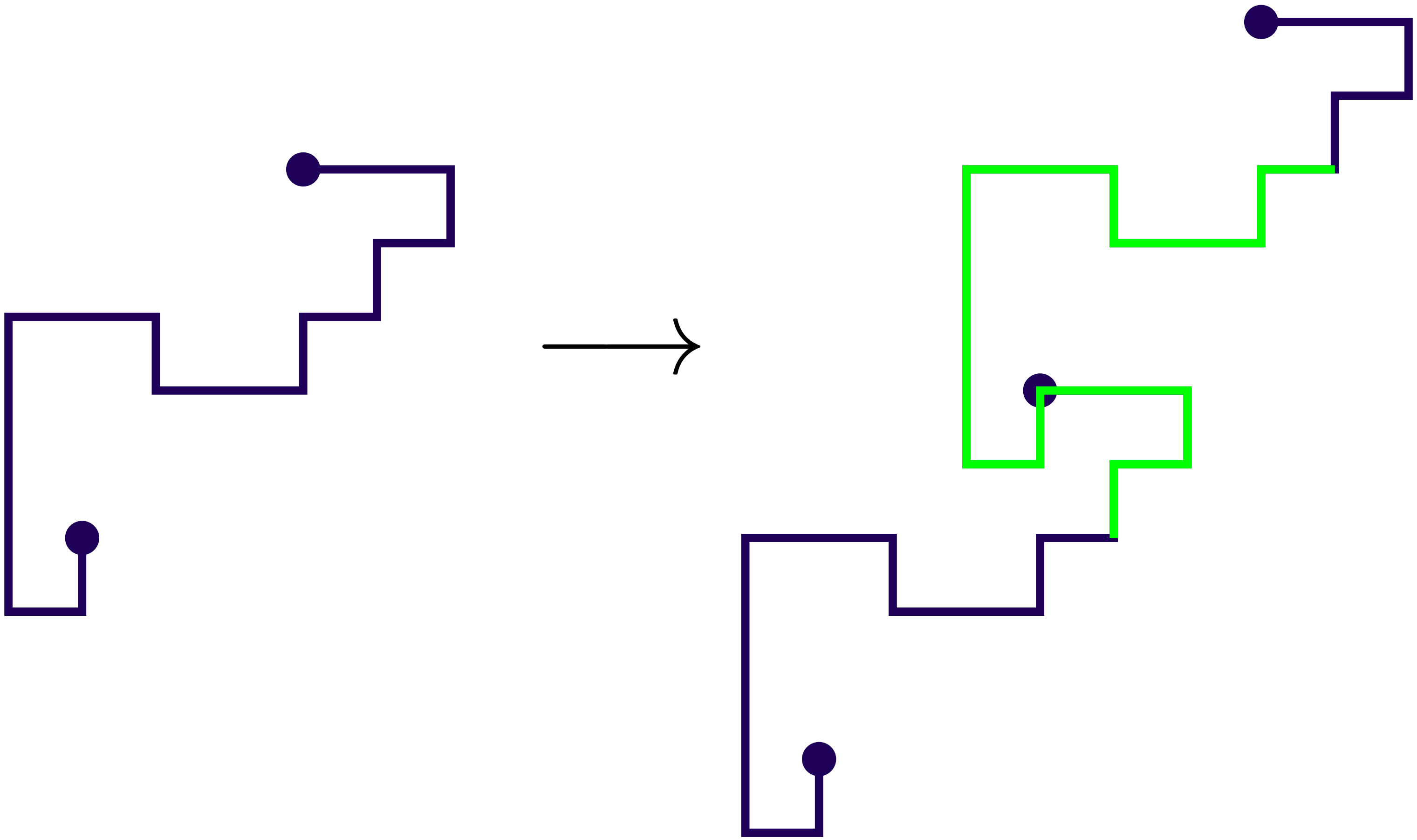
$$I(z) = 1 - \frac{1}{B(z)}$$



Endless bridge

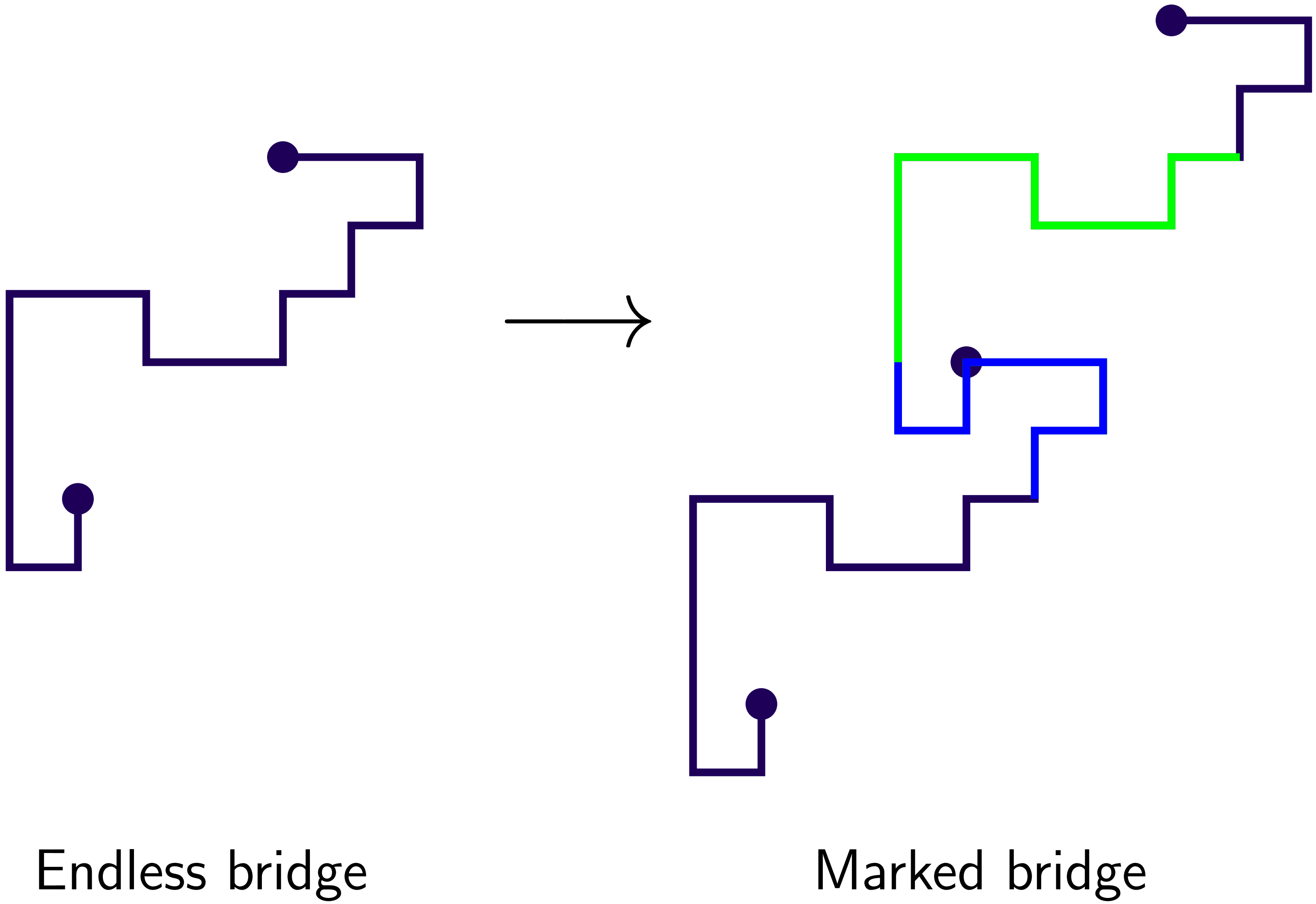


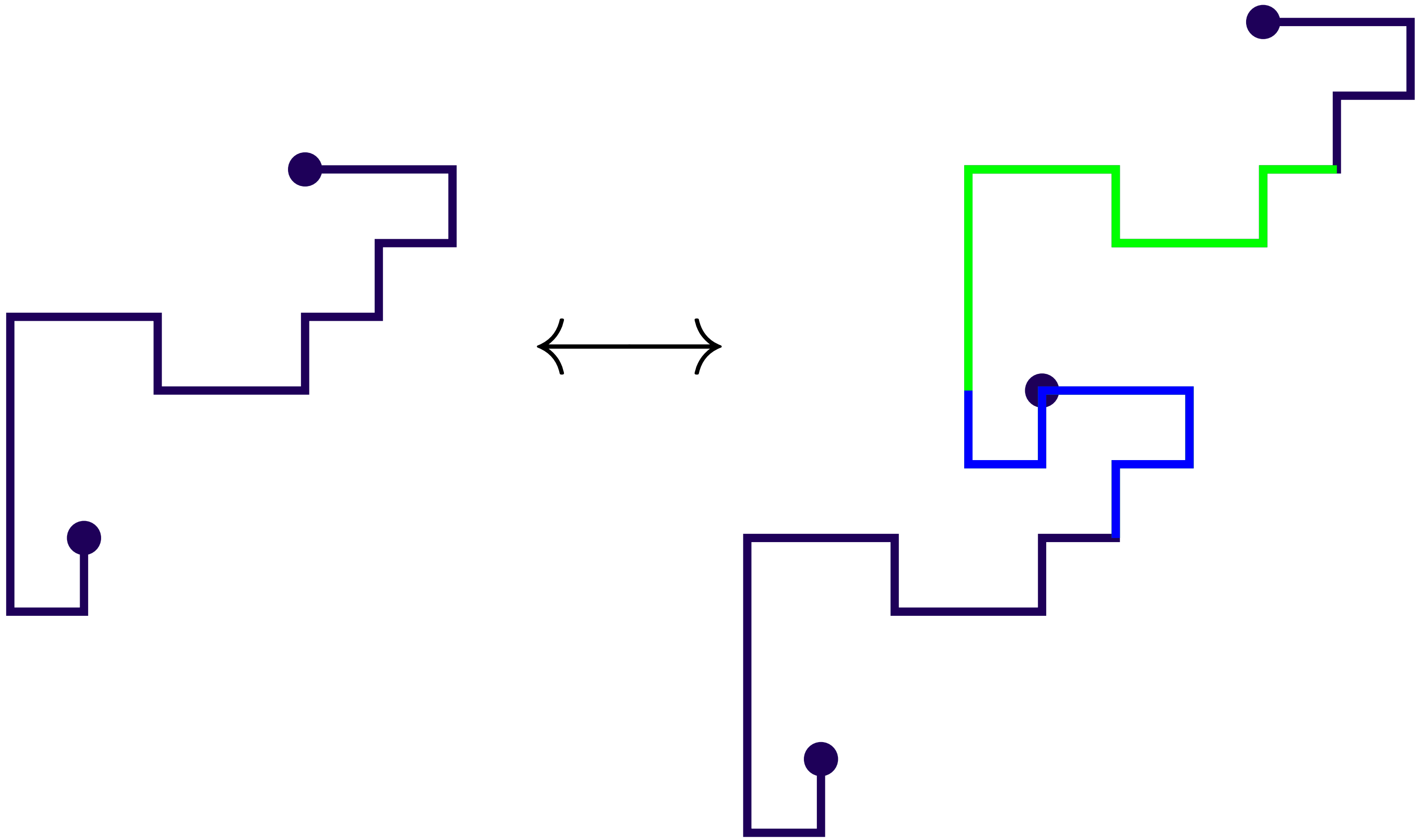
Endless bridge Marked bridge



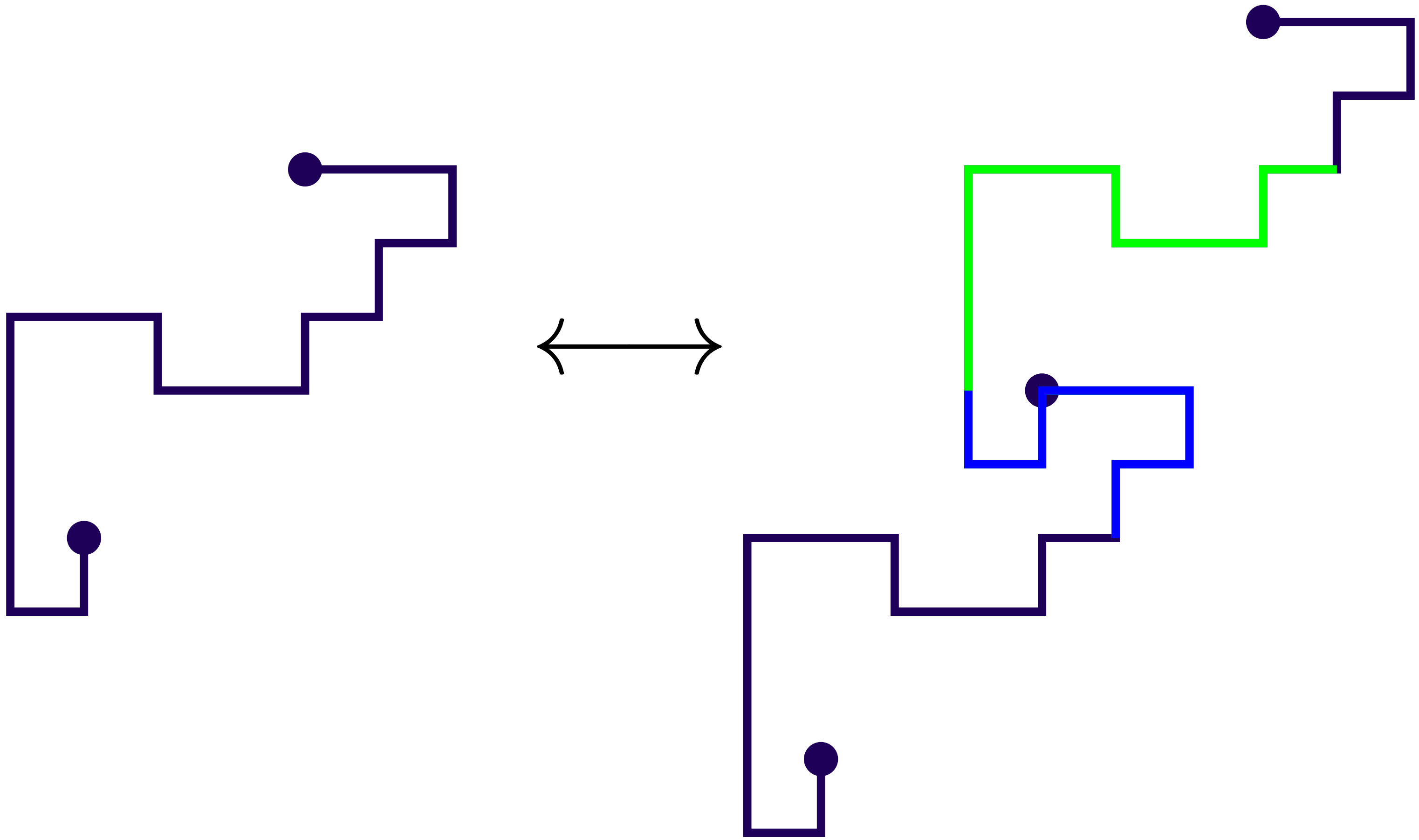
Endless bridge

Marked bridge


Endless bridge
Marked bridge



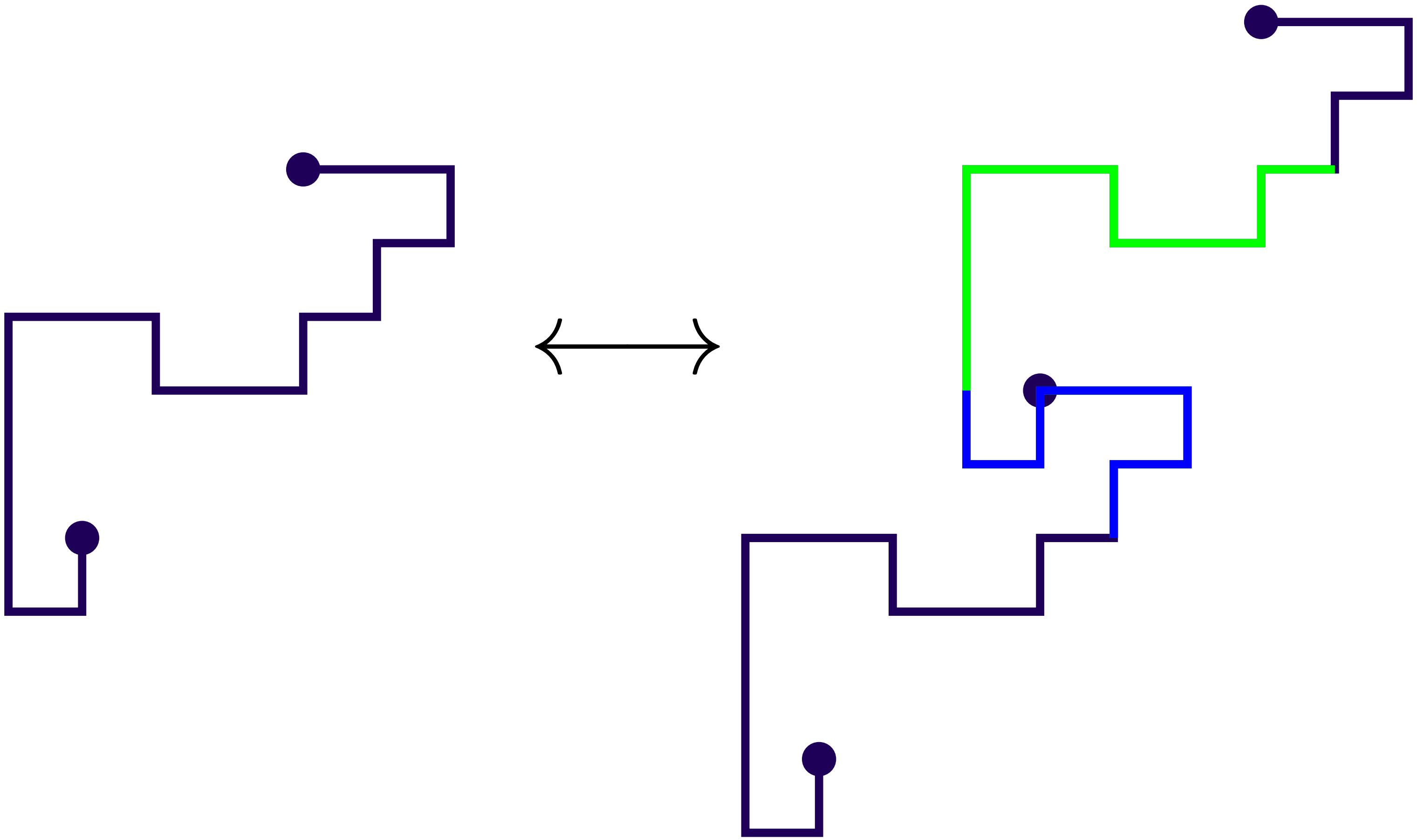
Endless bridge Marked bridge



Endless bridge

$EB(z)$

Marked bridge



Endless bridge

$EB(z)$

Marked bridge

$zI'(z)\ B(z)$

Bridges

The start point of any endless bridge must occur within an irreducible bridge, and the remainder of the endless bridge is either empty or an arbitrary bridge.

$$\begin{aligned} EB(z) &= zI'(z)B(z) = z(1 - B(z)^{-1})'B(z) \\ &= \frac{zB'(z)}{B(z)} \end{aligned}$$

Bridges

There is strong theoretical and numerical evidence that

$$b_n \sim A_b n^{\gamma_b} \mu^n$$

$$B(z) \sim \frac{A_b}{\Gamma(\gamma_b)} (1 - z/z_c)^{-\gamma_b}$$

$$B'(z) \sim \frac{\gamma_b}{z_c} \frac{A_b}{\Gamma(\gamma_b)} (1 - z/z_c)^{-\gamma_b - 1}$$

where γ_b is the bridge exponent and has value $9/16$ for $d = 2$, and $0.19835(3)$ for $d = 3$, and $z_c = 1/\mu$.

Therefore

$$EB(z) = \frac{zB'(z)}{B(z)} \sim \frac{\gamma_b z/z_c}{1 - z/z_c}$$

$$eb_n = \gamma_b \mu^n (1 + o(1))$$

Endless bridges are a positive fraction of eSAWs

We have

$$\begin{aligned} e_n &= A_e \mu^n (1 + o(1)) \\ eb_n &= \gamma_b \mu^n (1 + o(1)) \\ \implies \frac{eb_n}{e_n} &= \frac{\gamma_b}{A_e}(1 + o(1)) \end{aligned}$$

and so a positive fraction of eSAWs are in fact endless bridges!

eSAWs are, in some sense, a natural generalisation of bridges.

A technical aside

Bridges will drift in the positive y-direction, but they will also have break edges if they drift in the negative y-direction.

We do not care about the drift direction!

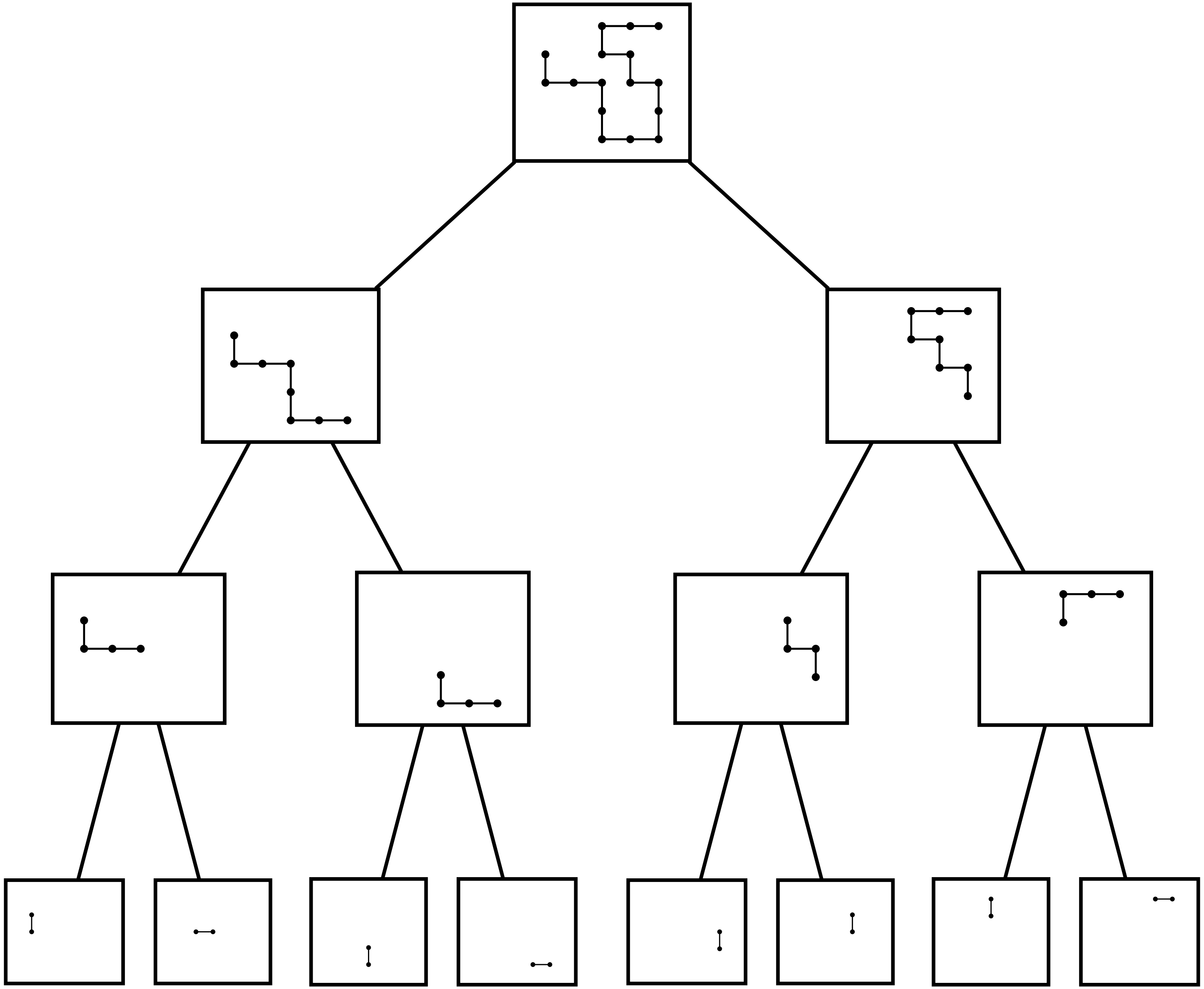
It means that

$$\Pr(\text{break edge}) = \frac{2eb_n}{e_n} = \frac{2\gamma_b}{A_e}(1 + o(1))$$

Detecting break edges efficiently

We need an efficient algorithm for detecting break edges, to determine if an eSAW is an endless bridge.

For the pivot algorithm, we have an efficient binary tree data structure that tracks “bounding box” information about the walk at different length scales.



SAW-tree representation of a walk.

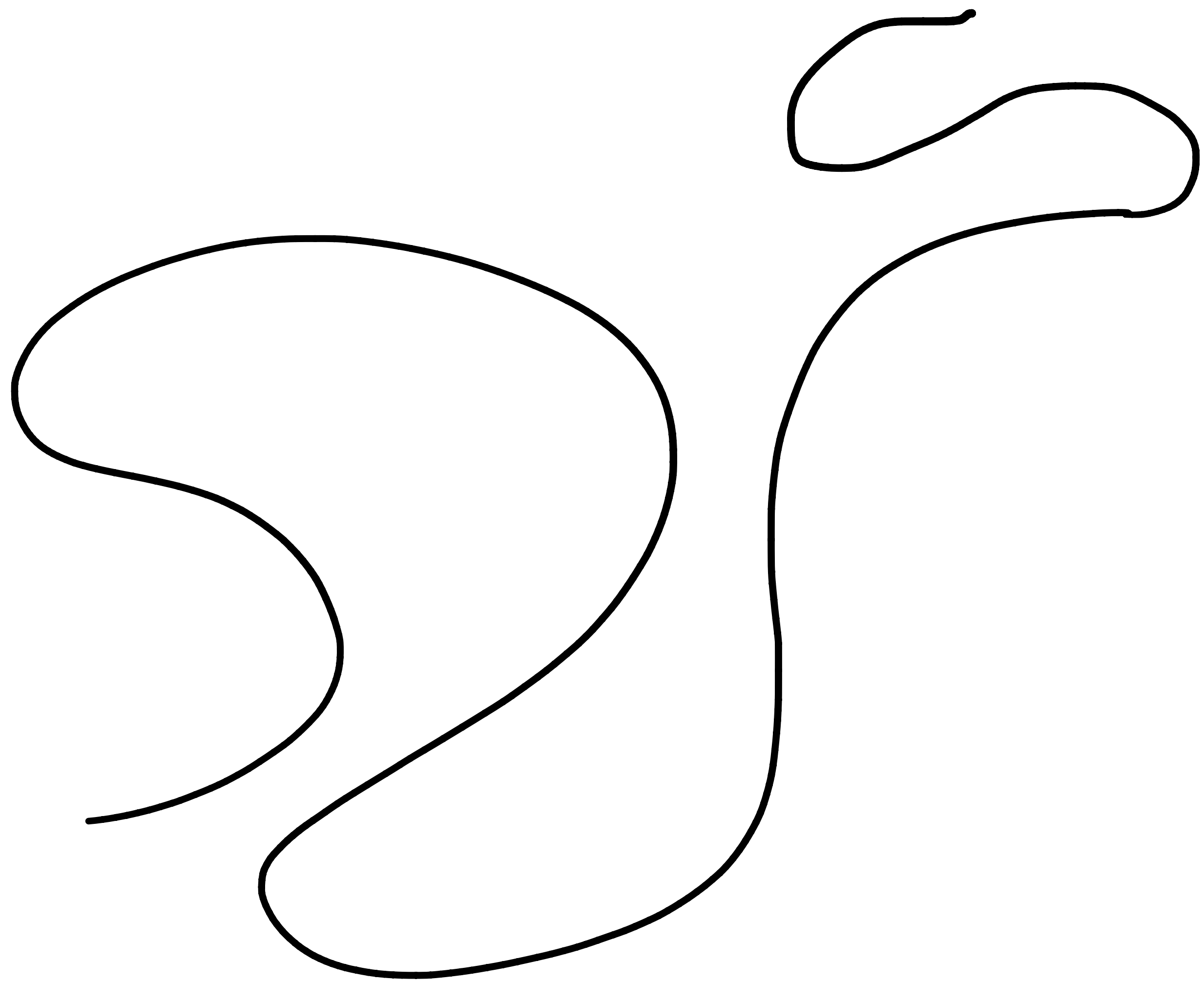
Detecting break edges efficiently

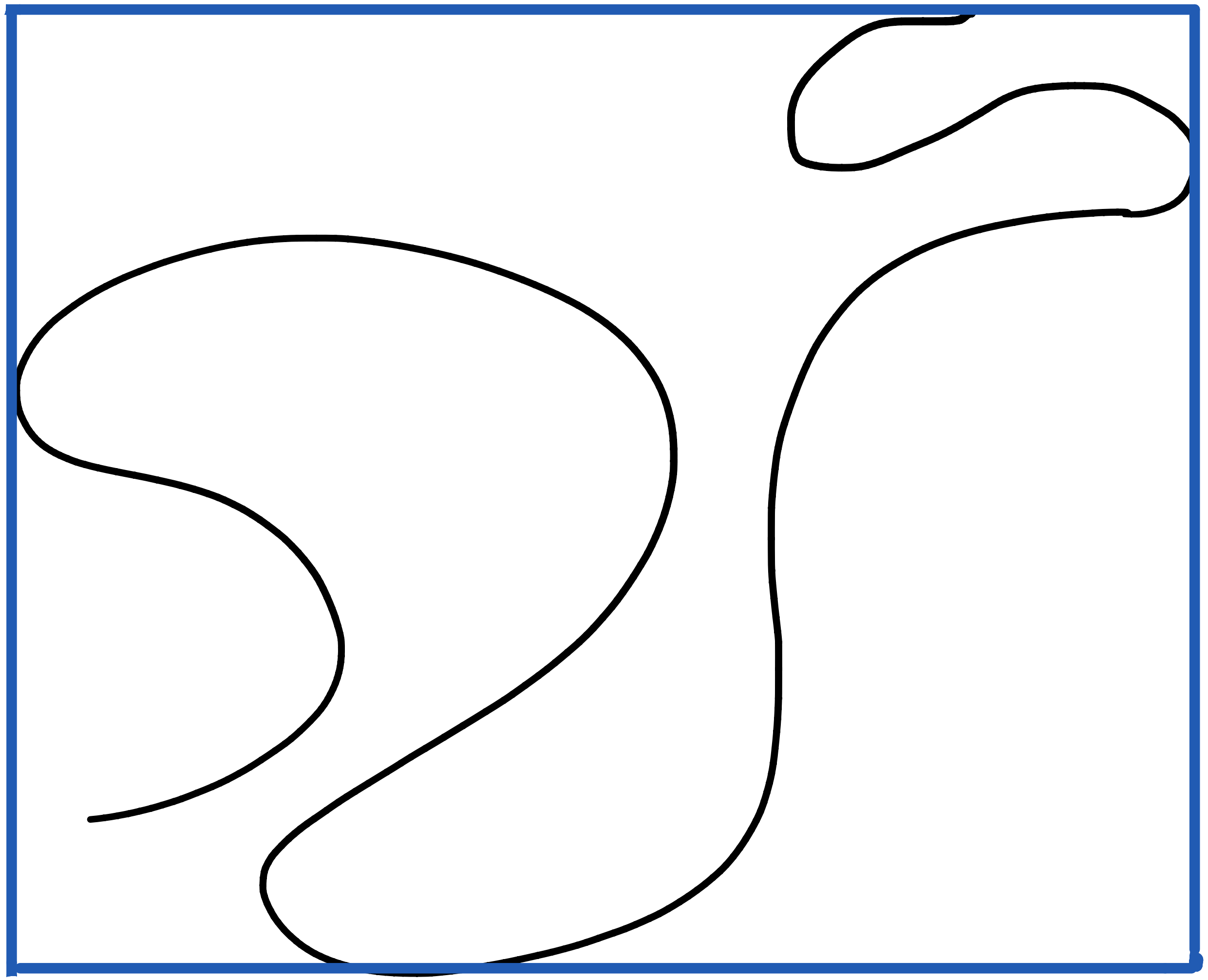
We can use the bounding boxes by exploiting the following facts:

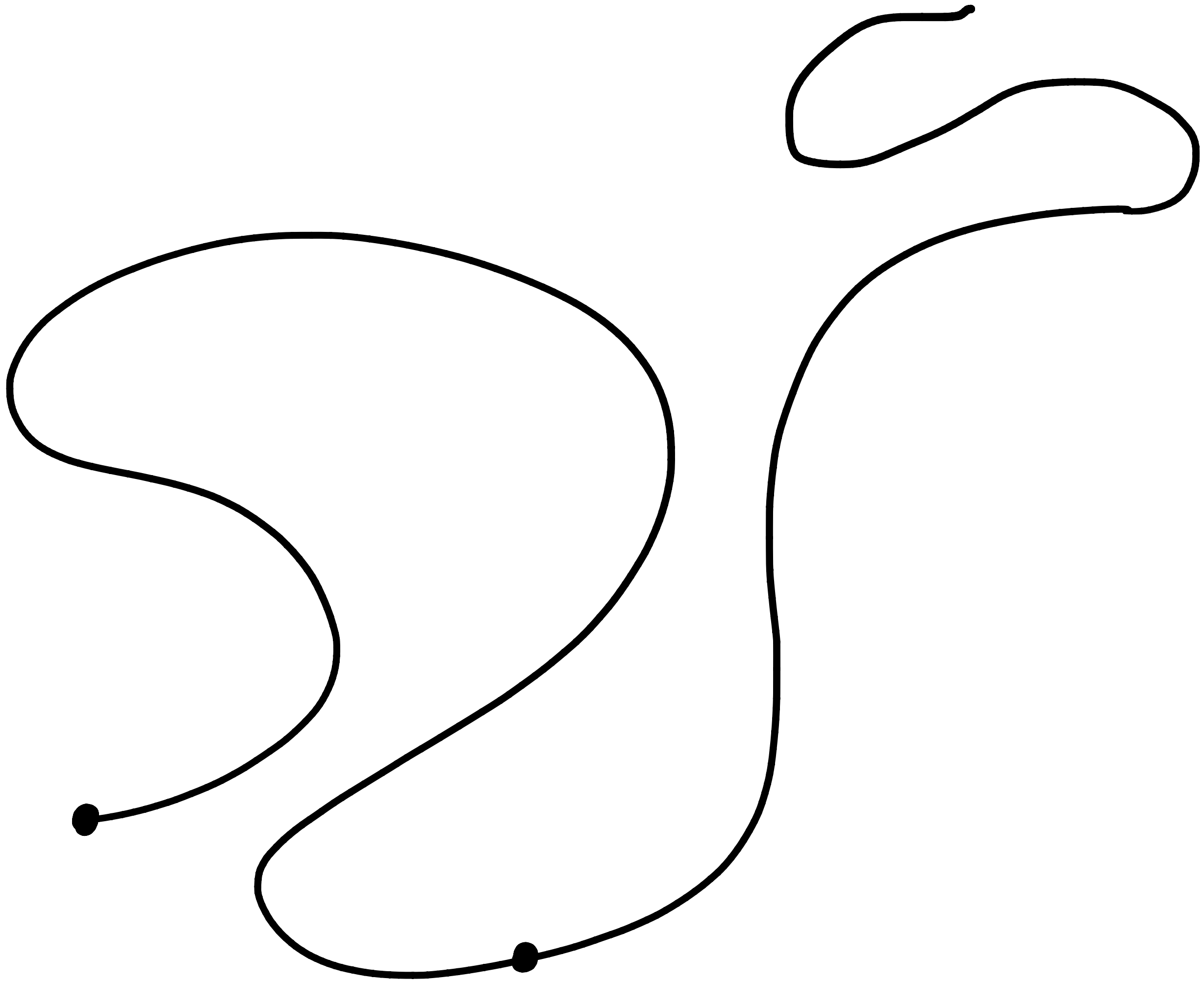
- Subwalks span their bounding boxes in all directions.
- If the projections of bounding boxes overlap, then necessarily there must be at least two spanning paths in the overlap and there cannot be a break edge.
- If bounding boxes are non-overlapping then there must be a break edge between them.

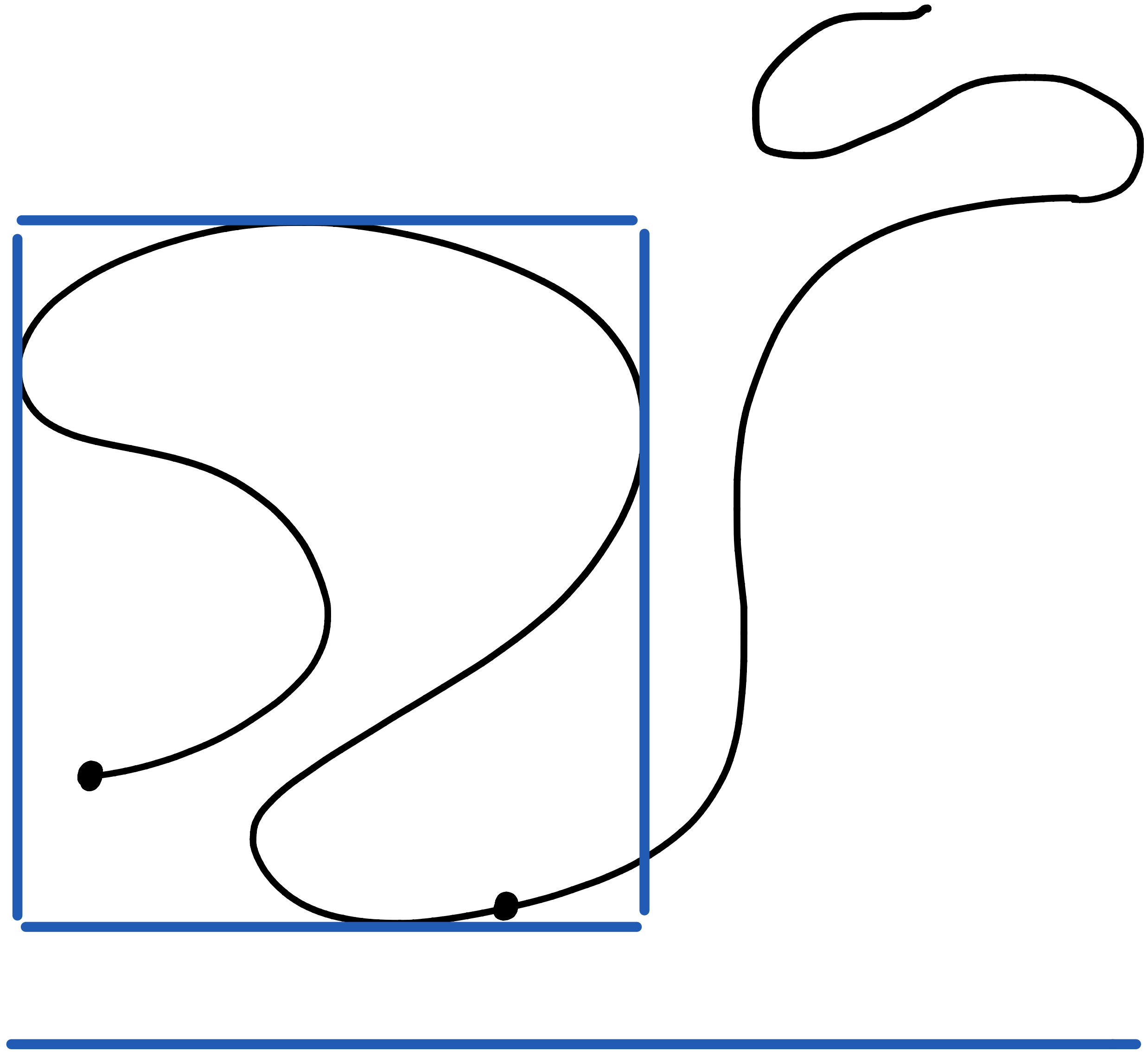
The algorithm proceeds by successively excluding regions as having break edges.

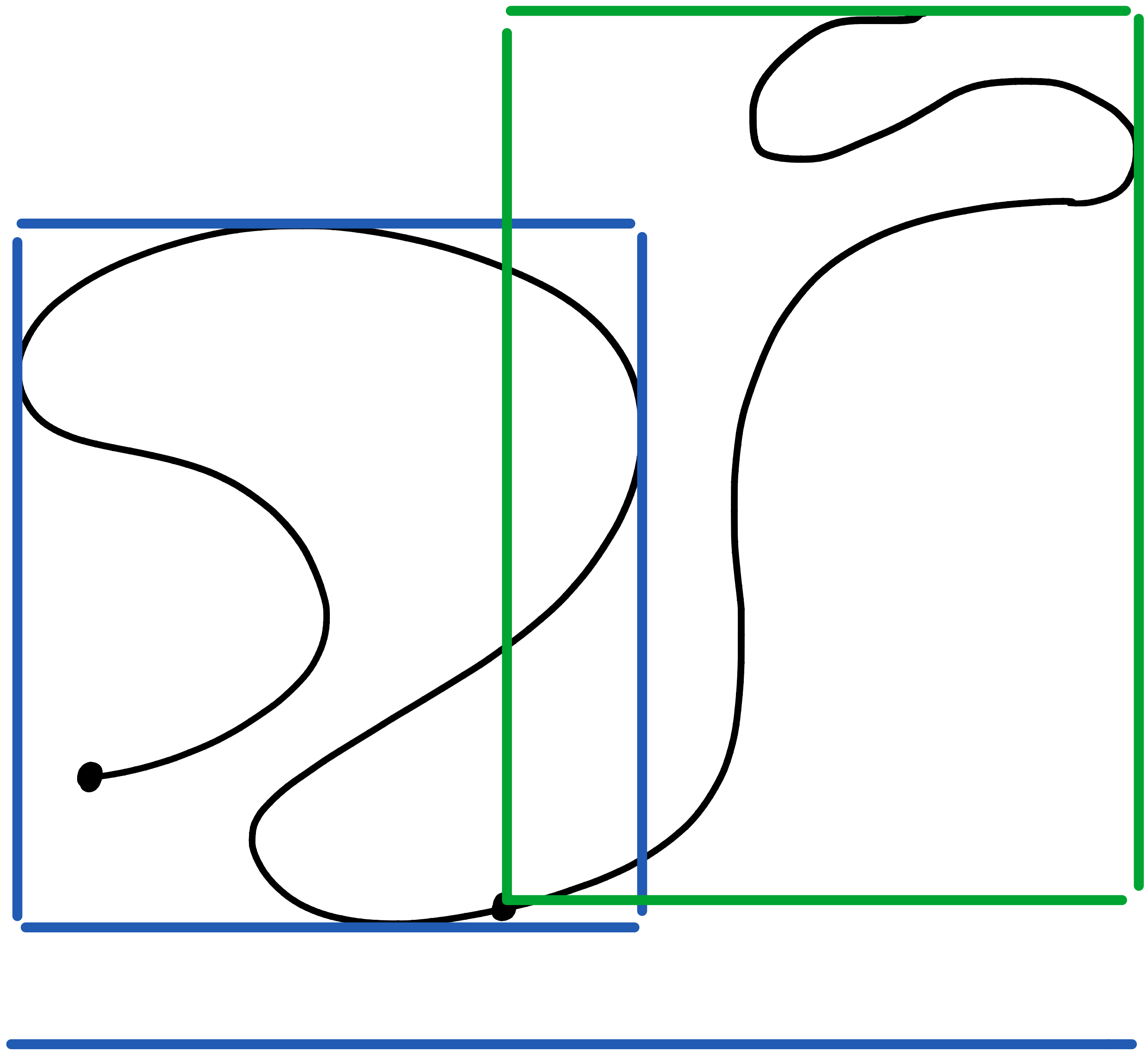
A break edge is detected when we have non-overlapping bounding boxes with an edge between them.

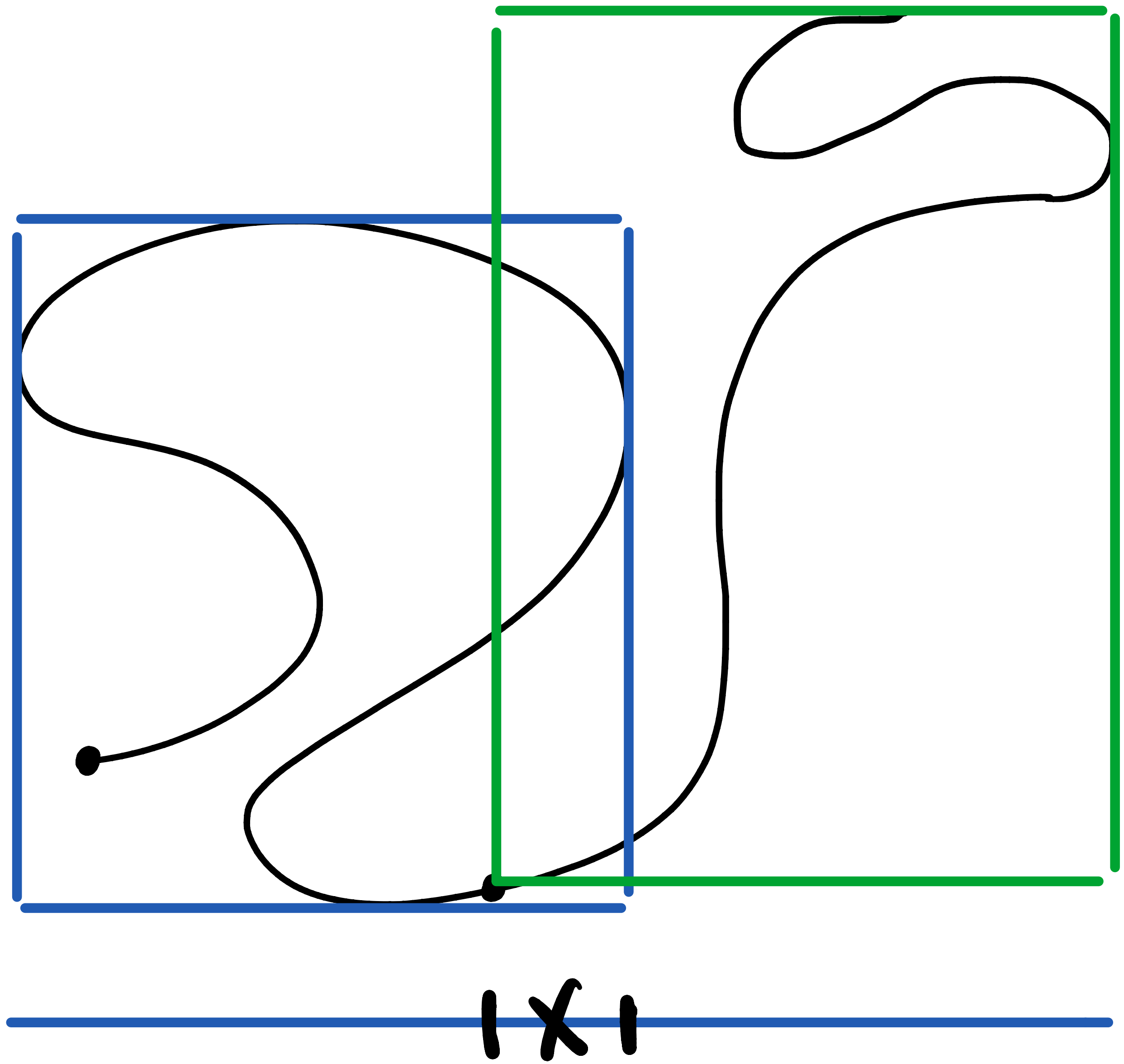


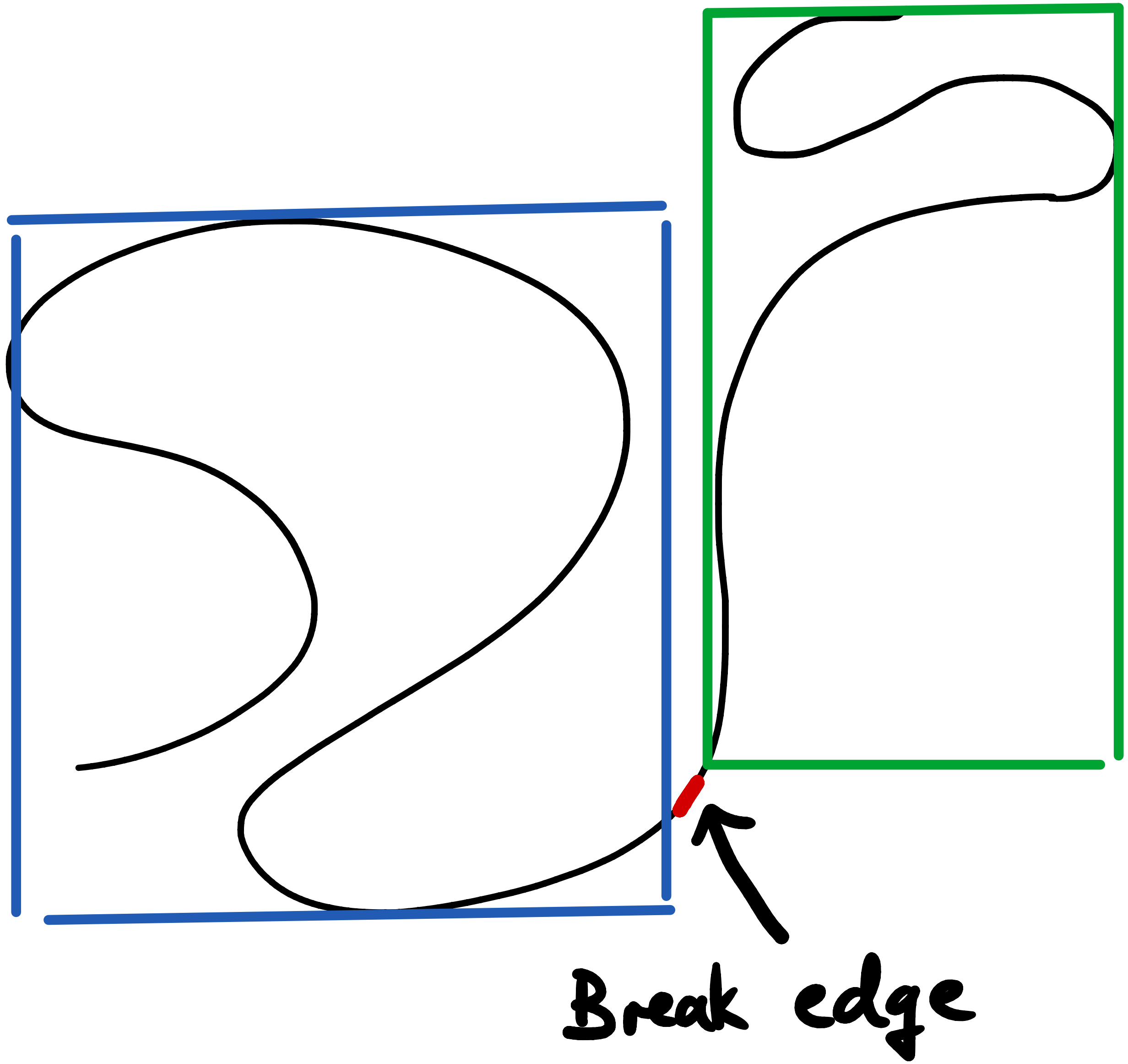









1x1


Break edge

Detecting break edges efficiently

The break edge detection algorithm appears to take average case time $O(\log N)$ to determine that there are no break edges, or to detect a single break edge.

It can also be adapted to count break edges instead.

Bridge data

We have sampled both SAWs (via pivot) and eSAWs (via modified pivot).

Sampling SAWs is more efficient, even though only a small proportion of them are eSAWs.

(We need a better version of the pivot algorithm for eSAWs!)

Computer experiment for N from 200 to 100 million.

Analysis

We try to extract as much information from our data as possible by fitting as many correction-to-scaling terms as possible.

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As a consequence, we cannot fit/model our first unfitted correction!

Hence, even if we are being careful, there will always be untested assumptions, both for Monte Carlo and series data.

Analysis

Here's some wisdom from Tony that I always keep in mind, referring to estimates derived from series analysis, in Asymptotic Analysis of Power-Series Expansions:

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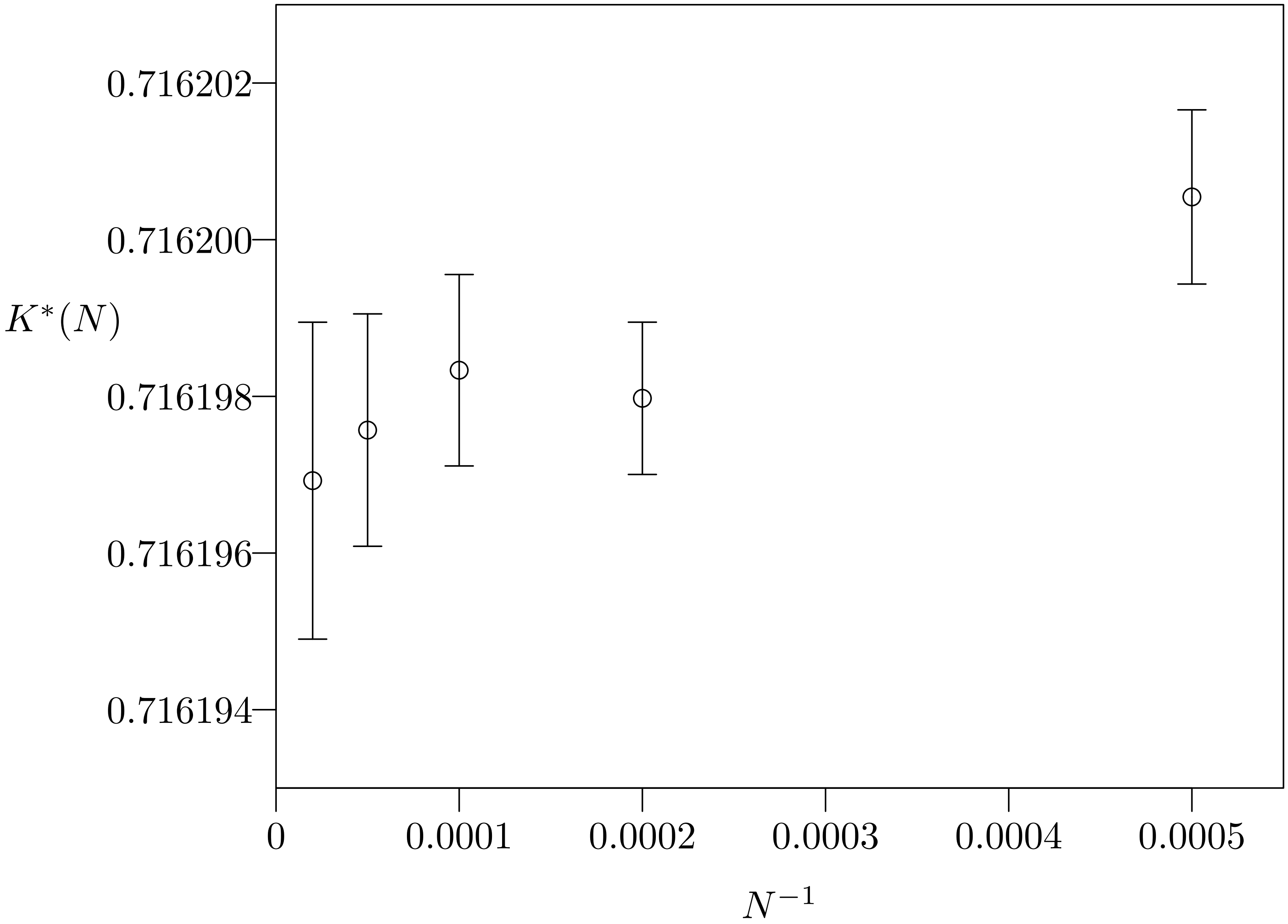
> *. . . error bounds are generally referred to as (subjective) confidence limits, and as such frequently measure the enthusiasm of the author rather than the quality of the data.*



Estimate of amplitude from biased fit.

We get 0.716197(3) vs predicted value of 0.71619724 . . .

eSAW amplitude

For SAWs in $d = 2, 3$ we have

$$c_n = An^{\gamma-1}\mu^n(1 + o(1)),$$

where A and μ are lattice dependent, and $\gamma = 43/32$ for $d = 2$ and $\gamma = 1.156953(1)$ for $d = 3$.

All eSAWs are SAWs, and so we can sample SAWs and estimate the probability that a SAW is an eSAW.

$$\Pr(\text{SAW is eSAW}) = \frac{e_N}{c_N} = \frac{A_e\mu^N(1 + o(1))}{AN^{\gamma-1}\mu^N(1 + o(1))} = \frac{A_e}{AN^{\gamma-1}}(1 + o(1))$$

We can use this relation to estimate γ and A_e.

eSAW amplitude data

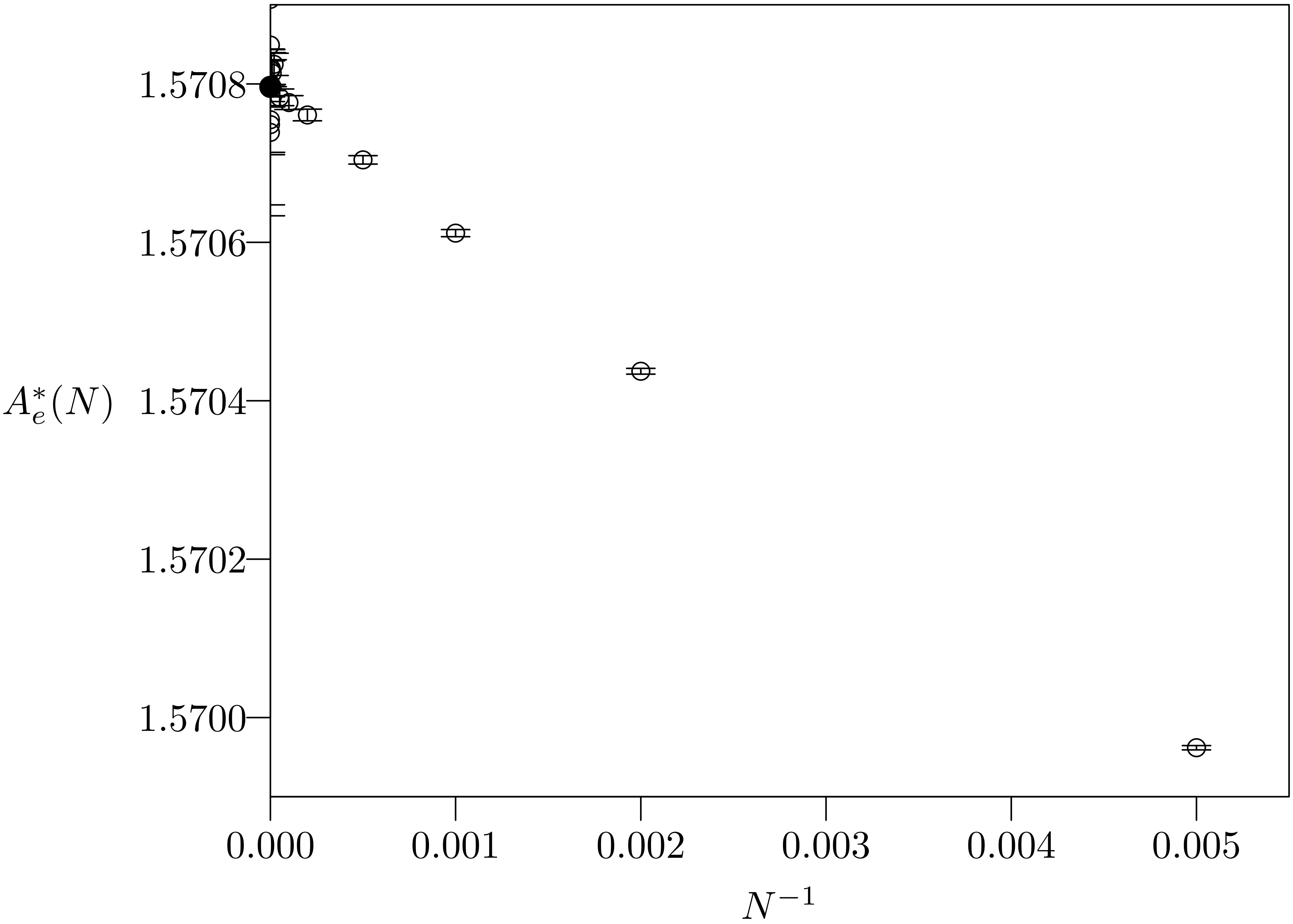
First we will plot

$$A_e^{(N)} = \Pr(\text{SAW is eSAW})\, AN^{\gamma-1}$$

where we expect that

$$A_e = \Pr(\text{SAW is eSAW})\, AN^{\gamma-1}\left(1 + \frac{a}{N} + \cdots\right)$$

Computer experiment for N from 200 to 100 million.



$A_e^*(N)$
1.5708
1.5706
1.5704
1.5702
1.5700
0.000
0.001
0.002
0.003
0.004
0.005
N^{-1}

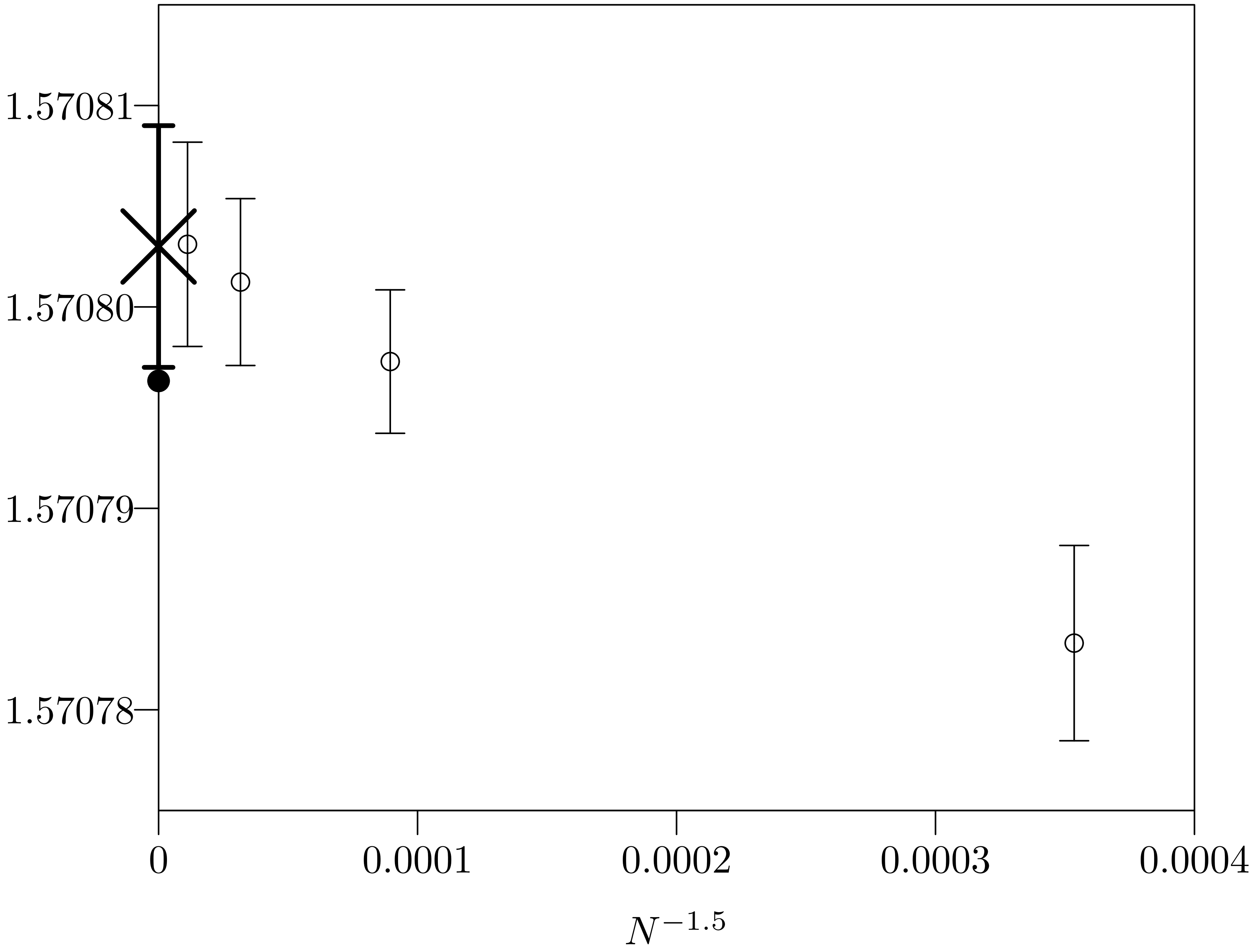
eSAW amplitude data

Next, we will assume that our scaling form is correct, and estimate A_e.

We can bias our fits by using the known value of γ to obtain an accurate estimate of A_e.

We fit the leading $1/N$ correction, and our largest neglected term is $O(N^{-3/2})$.

We plot our estimates against $N^{-3/2}$.


1.57081
1.57080
1.57079
1.57078
0
0.0001
0.0002
0.0003
0.0004
$N^{-1.5}$

eSAW estimates

Our best estimate is $A_e = 1.570803(6)$. (Estimate from enumeration data $A_e = 1.57075(10)$.)

Note: $\pi/2 = 1.570796326\cdots$.

We also obtain $\gamma = 1.3437492(25)$, compared with exact value of $43/32 = 1.34375$, and predictions from enumerations of $1.343745(5)$ due to Jensen.

For $d = 3$ we obtain $A_e = 1.18337(5)$. (Estimate from enumeration data $A_e = 1.183(3)$.)

We also obtain $\gamma = 1.1569505(25)$; previous Monte Carlo estimates are a little more accurate and give $1.156953(1)$.

Probability that eSAWs can be split or concatenated

We know that

$$\frac{e_{2N}}{e_N^2} \approx \frac{A_e \mu^{2N}}{A_e^2 \mu^{2N}} = \frac{1}{A_e}$$

We can sample eSAWs via the eSAW pivot algorithm.

We find the probability that an eSAW can be split into two eSAWs, and the probability that two eSAWs can be concatenated to form an eSAW.

Theory due to Duplantier allows these two exponents to be determined.

Exponents must be the same, as ratio of probabilities is the constant given above.

$\Pr(\text{split}) \sim C_1 N^y$, $\Pr(\text{join}) \sim C_2 N^y$, $y = \frac{\sqrt{31}}{8} - \frac{15}{16} = -0.24152945\ldots$.

Verified by computer experiment: $y = -0.2415305(20)$.

Conclusion and future work

- Joint work with Neal Madras.
- A positive fraction of eSAWs are endless bridges.
- eSAWs are, in some sense, a natural generalisation of bridges.
- A_e looks suspiciously close to $\pi/2$ for $d = 2$.
- More to be done for exactly solvable endless models and enumeration of eSAWs.
- Work in progress: a single site pivot move would dramatically improve the efficiency with which we can sample eSAWs.
- Unclear to me whether there will be ongoing applications of eSAWs due to their nice features, or if this is an interesting and fun dead end.
- For now, there are more insights into SAWs and polymer models to be discovered.