# Linear Cellular Automata via de Bruijn Diagrams

Harold V. McIntosh
Departamento de Aplicación de Microcomputadoras,
Instituto de Ciencias, Universidad Autónoma de Puebla,
Apartado postal 461, 72000 Puebla, Puebla, México.
E-mail:mcintosh@servidor.unam.mx

August 10, 1991

**Abstract**

Graph theory plays several important roles in the theory of cellular automata, one of which consists in describing the evolution of the automaton, and another of which consists in relating local properties to global properties. Evolution is described by local rules mapping cell neighborhoods into its subsequent state; because successive neighborhoods overlap it is important to be able to take the overlap into account when relating the behavior of successive cells to one another. In illustration, the de Bruijn diagram and its subdiagrams are applied to the study of cellular automata in one dimension.

## 1 Introduction

An automaton has *states* and *mappings* between its states. The concept arose from electrical switching theory, but thanks to the pioneering work of Claude Shannon [1], boolean algebra and probability theory were seen to have an important role in the theory of switching networks. Speculation concerning the relationship between logical processes and the physiology of the nervous system, modelled by networks of cells, had early origins in the work of Warren McCulloch and Walter Pitts [2]. Numerous subsequent investigators have contributed to the subject, in forms ranging all the way from abstract mathematical logic and formal language theory to concrete engineering and biological simulations and experiments.

A *cellular* automaton lends itself to rigorous analysis because of the symmetry inherent in a crystallographic lattice of individual automata—the cells—and the assumption that individual changes of state depend solely on the states of a limited number of neighbors. At first sight the extensive overlapping between neighborhoods of different cells seemed to confuse the issue, but then it was

found that certain ideas used in shift register theory and various techniques from information theory took care of the overlapping in a very natural and elegant way.

Without going into the details of automata theory, our objective is to present graph theory from a point of view useful for automata theory, while also exhibiting some important theorems for this application.

# 2 Five representations

Graphs have varied representations, each of which has its advantages and its limitations.

## 2.1 Mathematical definition

From a purely abstract point of view, a graph is a pair $(N, L)$ consisting of *nodes* $N$ and *links* $L$. The nodes are just a set, often taken to be the positive integers from 0 to $n-1$; the links are a subset of $N \times N$

## 2.2 Simple drawing

The nodes are laid out as dots on a sheet of paper, frequently labelled by the members of the set $N$. The links are represented by arrows joining the nodes, the arrow runs *from* node $i$ *to* node $j$ if $(i,j) \varepsilon L$. Note that there is no requirement that both $(i,j)$ and $(j,i)$ belong to $L$, nor that $(i,i)$ either belongs or does not belong.

It is a classical problem in graph theory, to decide whether a graph may be drawn in two dimensions so that its links do not cross; this point does not interest us except insofar as the aesthetics of laying out the graph is concerned.

## 2.3 Topological matrix

The topological matrix $M_{ij}$ is defined by

$$M_{ij} = \begin{cases} 1 & (i,j) \varepsilon L \\ 0 & \text{otherwise} \end{cases}$$

The most important application of the topological matrix consists in the fact that its powers describe paths between nodes containing multiple links, according to the power involved. Since the elements of such matrices are integers the powers are useful for counting total numbers of paths, but not to classifying the paths into different categories. The reason for this is apparent from examining

the definition of matrix multiplication,

$$\begin{aligned}[M]^2_{ij} &= \sum_k M_{ik}M_{kj} \\ &= \sum_k \text{link}(ik)\text{link}(kj) \\ &= \sum_k \text{link}(ikj).\end{aligned}$$

Diagonal elements of this matrix count loops; the trace yields the total number of loops, counting each of them once for every node which they contain. Thus

$$\begin{aligned}\phi(t) &= \sum_{n=1}^{\infty} \frac{t^n}{n}\text{Trace}(M^n) \\ &= -\text{Trace}(\ln(I - tM)).\end{aligned}$$

is a generating function for the prime loop count. By prime loop is meant one for which portions of the loop are not retraced. By using a determinantal identity for the matrix exponential, it is possible to obtain a generating function involving the characteristic equation of $M$ (and using a matrix version of $\phi$).

$$\begin{aligned}\zeta(t) &= \text{Det}(e^{\phi(Mt)}) \\ &= \text{Det}(I - tM)^{-1} \\ &= \chi(t)^{-1},\end{aligned}$$

where $n$ is the dimension of $M$ and $\chi$ is its characteristic polynomial. Actually this is a variant definition of the characteristic polynomial, often seen in integral equation theory; by associating $t$ with $M$ rather than $I$ the limit of large $n$ is better behaved.

## 2.4 Symbolic equations

To describe a graph symbolically, let the nodes be represented by variables, such as the capital letters $X$, $Y$, $Z$, and the links by constants, such as the lower case letters $a$, $b$, $c$. *Entrance equations* for the graph may be written in the form

$$X = Ya + Zb + \lambda$$

which say that one arrives at the node $X$ by having previously arrived at the node $Y$ and then following the link $a$, by having arrived at $Z$ followed by $b$, or by simply remaining at the node $X$. The latter alternative is used when $X$ is a terminal point, otherwise the term $\lambda$ would be dropped from the equation.

Conversely *exit equations* take the form

$$X = aY + bZ + \lambda$$

with $\lambda$ marking initial nodes. In either event, the entire diagram is described by a system of equations which can be written in the appropriate symbolic matricial form,

$$\begin{aligned} \mathbf{M} &= \mathbf{AM} + \mathbf{R} \\ \mathbf{M} &= \mathbf{MA} + \mathbf{R}, \end{aligned}$$

whose symbolic matricial solutions according to Arden's lemma,

$$\begin{aligned} \mathbf{M} &= \mathbf{A}^*\mathbf{R} \\ \mathbf{M} &= \mathbf{R}\mathbf{A}^*, \end{aligned}$$

have been described by John Conway [3], and in considerably greater detail by Backhouse and Carré [4]. The essence of the method consists in a recursive application of the identity

$$\begin{bmatrix} A & B \\ C & D \end{bmatrix}^* = \begin{bmatrix} \alpha & \beta \\ \gamma & \delta \end{bmatrix},$$

to a suitably partitioned $\mathbf{A}$, where

$$\begin{aligned} \alpha &= (A^*BD^*C)^*A^* \\ \beta &= (A^*BD^*C)^*A^*BD^* \\ \gamma &= (D^*CA^*B)^*D^*CA^* \\ \delta &= (D^*CA^*B)^*D^*. \end{aligned}$$

Trying to split $\mathbf{A}$ in half is an efficient way to reduce the amount of calculation required; removing the first row and column yields very tractable iterative formulas. Alternatively, rewriting $\mathbf{A}$ as a sum via sundry regular expression identities yields analogues of the LR factorization of matrices, wherein the stars of triangular factors are much easier to compute than for full matrices.

## 2.5 Regular expression

The solutions of linear symbolic equations are regular expressions, which represent sets. In other words regular expressions furnish a concise description of the paths through a diagram rather than the diagram itself. Comparisons between regular expressions therefore translate into comparisons between the sets which they represent, and conversely. As a result, boolean operations such as intersection and complementation are possible on regular expressions; union already forms part of the algebra of regular sets.

Likewise, due to the distributive and associative laws, it is possible for diverse regular expressions to represent the same set, creating the problem of recognizing the equality of two different regular expressions.

# 3 Comparison of diagrams

One can discuss the ordering and the equivalence of diagrams. From the first, one might stipulate that one diagram is larger than another if it has all the nodes of the smaller; likewise all the links. If $D_1 = (N_1, L_1)$ is one diagram and $D_2 = (N_2, L_2)$ is another, then $D_1 \leq D_2$ would mean

$$N_1 \subset N_2 \text{ and } L_1 \subset L_2.$$

In short, subdiagrams would be smaller. However we are also interested in comparing paths through diagrams, and not necessarily the diagrams themselves. So mappings between diagrams could hold our interest because of wanting to embed a given path in an equivalent diagram which could be more favorable.

There are many other reasons for such an interest in mappings. Drawings can be laid out quite differently as the groupings of nodes are changed or the crossing of links is avoided; regular expressions can be rearranged according to the distributive and associative laws, and so on. At the very least, mappings between different formulations are desirable, to be able to compare them to one another, and to recognize equivalent formulations.

## 3.1 Order relation

Consequently a more general point of view might hold that the larger graph contains all the paths of the smaller, especially the loops. Actually, the image of a loop has to be a loop because any point of closure has the same image as the point of departure; but additional loops may exist in the image. To repeat, we want to say that a larger graph has more paths, even if they are degenerate; such a viewpoint is still consistent with embedment into a graph that the first sense considers larger.

Consider (writing ab for (a,b) whenever it is unambiguous to improve legibility)

$$\{a, b; ab, ba\}$$

and

$$\{a, b, c, d; ab, bc, cd, da\};$$

these graphs are diagrammed in Figure 1.

The second, larger, is a digon with its vertices linked to one another; the first, smaller, is a square with successive vertices linked. Mapping a to a, b to b, c to a, and d to b, it is seen that cycles around the square runs twice around the digon, with similar relationships for other paths.

The interesting point is that the larger is not a superset of the larger, but rather it contains a functional image. One might say that $D_1 \leq D_2$ means that

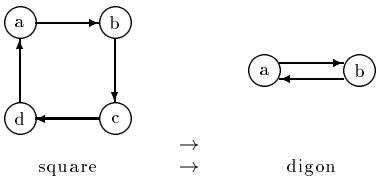



Figure 1: A digon is larger than a square, which has no loops of length 2.

there exists a function such that

$$\begin{aligned} f(N_1) &\subseteq N_2 \\ \text{link}(a,b) &\Rightarrow \text{link}(f(a),f(b)) \end{aligned}$$

This definition reduces to the previous one when $f$ is the injection map that inserts a subset into the set containing it, but allows a comparison which extends far beyond pairs of diagrams in which one is a subset of the other.

Strictly, it must be proved that this general comparison is an order relation. The only complicated point is proving antisymmetry, that when $f(X) \subseteq Y$ and $g(Y) \subseteq X$ (and links are conserved), $X$ and $Y$ are at least equivalent if not identical. The mapping $f(x) = 2x$ applied in succession to the integers, even integers, and the multiples of four shows that this need not be true in general, although it works out well enough for finite sets.

## 3.2 Least upper bound, or union

Consider the graphs

$$\{a, b; abba\}$$

represented by a digon, and

$$\{a, b, c; ab, bc, ca\}$$

represented by a triangle. The loops of the first have length 2, those of the second, length 3. It would seem that loops belonging to one or the other would belong to their union, in which links would exist if and only if they had already existed in the components.

$$(N_1, L_1) \cup (N_2, L_2) = (N_1 \cup N_2, L_1 \cup L_2)$$

The sense of inclusion in the definition of the order relation was chosen so that one of the two connected components could be ignored while making comparisons. In general, it is profitable to consider a graph as a union of its disconnected parts and to observe that conversely, nontrivial unions are disconnected.

The topological matrix of the union of two diagrams is the direct sum of the topological matrices of the constituents.

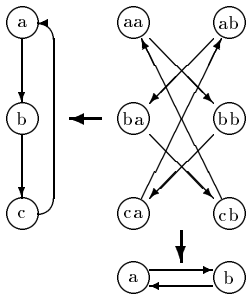



Figure 2: Greatest lower bound of a digon and a triangle.

### 3.3 Greatest lower bound, or intersection

Consider the same graphs,

$$\{a, b; ab, ba\}$$

representing a digon, and

$$\{a, b, c; ab, bc, ca\}$$

representing a triangle. The loops of the first have length 2, those of the second, length 3. It would seem that loops common to the two would have length 6; what is the diagram which would express this fact? The evident candidate is the cartesian product of the two graphs, linkage between its points occurring only if both coordinates were linked, for which we use the symbol $L_1 \sharp L_2$.

$$(N_1, L_1) \cap (N_2, L_2) = (N_1 \times N_2, L_1 \sharp L_2)$$

Effectively, linkage in the cartesian product is defined by

$$\text{link}((a, b), (c, d)) = \text{link}(a, c) \& \text{link}(b, d).$$

In this example, the intersection has nodes

$$\{(a, a), (a, b), (a, c), (b, a), (b, b), (b, c)\},$$

with links

$$\{((a, a), (b, b)), ((b, b), (a, c)), ((a, c), (b, a)),$$
$$((b, a), (a, b)), ((a, b), (b, c)), ((b, c), (a, a))\}.$$

Graphed by usual conventions, a folded hexagon results, manifesting the required cycle of length 6, as seen in Figure 2.

The topological matrix of the intersection of two diagrams is the tensor product of the topological matrices of the constituents.

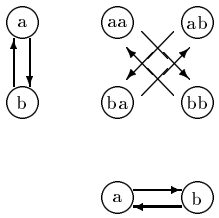



Figure 3: Greatest lower bound of a digon with itself.

# 4 Mappings and equivalences

As an interesting point, consider the proposition that a graph is the intersection of two copies of itself, yet the cartesian square or the tensor square of a diagram has quite a few more nodes. However they can be grouped into components, one single image of the graph repeated once for each node. A similar anomaly appears with the union of a graph with itself, both situations showing that the ordering is incompletely defined unless the role of functional mappings and equivalences is clearly understood.

To promote such an understanding, consider the cartesian product of the digon with itself. The nodes

$$\{(a,a),(a,b),(b,a),(b,b)\}$$

are linked by

$$\{((a,a),(b,b)),((b,b),(a,a)),$$
$$((a,b),(b,a)),((b,a),(a,b))\}$$

which are seen to form two independent digons; this is shown in Figure 3. Either of them can be mapped onto the original digon by one or another of various mappings, or the pair can be mapped in two to one fashion by either of the two coordinate projections.

Evidently graphs can have many representations, making it desirable to have ways of comparing them to one another; functional mappings among the nodes, which preserve linkage, provide a good mechanism.

## 4.1 Homomorphisms

A mapping from the nodes of one graph to those of another which preserves linkages is called a *homomorphism*, whose definition was already introduced while defining the ordering of graphs. In short, the larger graph is a homomorphic

image of the smaller, even though the scarcity of its nodes will run counter to this intuition.

However, there is a subtle point which concerns the mappings of non-links — should they also be respected? As stated, the definition allows a single node linked to itself to be the maximum of all graphs; the requisite mapping is simply a constant mapping. All images are thereby linked, even when their counterimages are not. Another instance where the difference is felt concerns the difference between equivalence relations and congruence relations.

Equivalence classes are the constant value contours of functions; congruence classes are contours of homomorphisms. It might be interesting to impose a uniformity requirement, such as stipulating that

$$if \begin{cases} a \equiv b \\ x \equiv y \end{cases} \quad then \quad \text{link}(a,x) \Rightarrow \text{link}(b,y)$$

In other words, links would always have to be uniform throughout congruence classes, but a moment's thought shows that this need not even be true for all cartesian products, where one would surely expect such a result to be valid. Uniformity would disallow too many reasonable non-links; if non-links as well as links had to be preserved, this congruence relation would characterize such a homomorphism.

A graph of the sort required, where every member of a set of $p$ elements is linked to all the members of a set of $q$ elements is traditionally named $K_{p,q}$; $K_{p,p}$ is simply $K_p$.

As homomorphisms have been defined, the only requirement which two congruence classes have to satisfy is that if their images are linked, at least one pair of representatives have to be linked; this is still enough of a requirement to distinguish between equivalences and congruences. Let $P$ and $Q$ be congruence classes; then

$$\text{link}(P,Q) \quad \equiv \quad (\exists p \in P, q \in Q) \ni \text{link}(p,q). \tag{1}$$

The discarded version would have read:

$$\text{link}(P,Q) \quad \equiv \quad (\forall p \in P, q \in Q)\text{link}(p,q). \tag{2}$$

A new diagram constructed from the congruence classes of another will have fewer nodes, still preserving the links of the original diagram. Such replacements are often sought, in the interest of economy. In the extreme case of a maximum congruence relation, the final graph will have a minimum number of nodes, a unique representation of the original diagram and all others homomorphic to it.

Consider again the intersection of two diagrams, while supposing that $(a,b) \equiv (c,d)$ means that $b = d$ and that $\text{link}((u,v),(w,x))$ means $\text{link}(v,x)$ with respect to equivalence classes. Then the projection $\pi_2(a,b) = b$ is a mapping from the intersection to its second factor whose equivalence classes correspond to the first

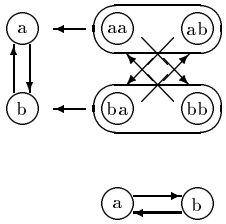



Figure 4: Congruence classes for the projection of a cartesian product onto its second coordinate; vertical components of links are respected.

factor; there is a similar projection $\pi_1$ for the first factor. Either is a congruence relation because the mapping is defined uniformly for the entire equivalence class. Figure 4 illustrates this relationship.

Note that there are no links within a single congruence class, as a consequence of which there are no self-loops in the projection.

## 4.2 Matrix representation

A rectangular matrix can represent a mapping between the nodes of one diagram and another; each column belonging to a node will have nonzero elements in the rows corresponding to the nodes mapping into it. In fact, the rows will be either orthogonal or identical, according to whether images are different or equal. The following relation is the matrix version of the mapping of a square to a digon shown in Figure 1:

$$\begin{bmatrix} . & 1 & . & . \\ . & . & 1 & . \\ . & . & . & 1 \\ 1 & . & . & . \end{bmatrix} \begin{bmatrix} 1 & . \\ . & 1 \\ 1 & . \\ . & 1 \end{bmatrix} = \begin{bmatrix} . & 1 \\ 1 & . \\ . & 1 \\ 1 & . \end{bmatrix}$$

$$= \begin{bmatrix} 1 & . \\ . & 1 \\ 1 & . \\ . & 1 \end{bmatrix} \begin{bmatrix} . & 1 \\ 1 & . \end{bmatrix}.$$

Likewise the mapping of the cartesian product shown in Figure 4 takes the form:

$$\begin{bmatrix} . & . & . & 1 \\ . & . & 1 & . \\ . & 1 & . & . \\ 1 & . & . & . \end{bmatrix} \begin{bmatrix} 1 & . \\ 1 & . \\ . & 1 \\ . & 1 \end{bmatrix} = \begin{bmatrix} . & 1 \\ . & 1 \\ 1 & . \\ 1 & . \end{bmatrix}$$

$$= \begin{bmatrix} 1 & . \\ 1 & . \\ . & 1 \\ . & 1 \end{bmatrix} \begin{bmatrix} . & 1 \\ 1 & . \end{bmatrix}.$$

Link imaging is built into the matrix equation; the test of whether the mapping is a homomorphism is that the product matrix resemble the connectivity matrix of the image diagram, as determined by the respective arrangements of the nonzero elements. For example, if nodes $a$, $b$, and $c$ of the square of Figure 1 were mapped into node $a$ of the digon with node $d$ mapping into node $b$, the equation above would become:

$$\begin{bmatrix} . & 1 & . & . \\ . & . & 1 & . \\ . & . & . & 1 \\ 1 & . & . & . \end{bmatrix} \begin{bmatrix} 1 & . \\ 1 & . \\ 1 & . \\ . & 1 \end{bmatrix} = \begin{bmatrix} 1 & . \\ 1 & . \\ . & 1 \\ 1 & . \end{bmatrix}$$

$$\begin{bmatrix} 1 & . \\ 1 & . \\ 1 & . \\ . & 1 \end{bmatrix} \begin{bmatrix} . & 1 \\ 1 & . \end{bmatrix} = \begin{bmatrix} . & 1 \\ . & 1 \\ . & 1 \\ 1 & . \end{bmatrix}.$$

The discrepancy in the $(1,1)$ element of the products is due to $a$ linking to $b$ in the square, then mapping to $a$ in the digon; alternatively it maps to $a$ in the digon which can only link to the digon's $b$.

In mnemonic form, the matrix representation of a homomorphism is

$$\sum_l \text{link}(i,l)(f(l)=j) \leq \sum_l (f(i)=l)\text{link}(l,j),$$

normalized according to taste. Notice how the rows of the lefthand matrix scan the nodes of the source diagram to see if there are any links to be followed. The right hand side jumps directly to the destination to see whether there are any links that will complete a commutative diagram. The inequality supposes that additional links may form bridges. The combination definitely favors the $\exists$ version of the congruence relation.

In matrix form, the criterion for a homomorphism from the graph whose connectivity matrix is $A$ to that whose matrix is $B$ is for there to exist a conformable matrix $X$ such that

$$AX \quad \leq \quad XB. \tag{3}$$

In either of these formulations, inequality is sufficient to ensure the existence of links in the image set, but when equality prevails it means that there are no additional links in the image set. In other words, with equality both links and nonlinks are preserved.

It should be noted that inequality for nonnegative (indeed, arbitrary real) matrices is defined by requiring all corresponding pairs of matrix elements to satisfy the stated relationship. Generally, the matrix $X$ of Eq. 3, consisting of zeroes and ones, rectangular if the orders differ, describes the mapping between the nodes of the two graphs. Note that numerical inequality of the matrix elements follows the sense of the mapping: homomorphisms increase monotonically; the connectivity matrix of the larger graph (the one left multiplied by $X$) has larger matrix elements, even though it may have fewer nodes.

Although Eq.3 is extremely elegant, it is also capable of great mischief. Equality is the preferred condition, since it implies conservation of both links and non-links; however the definition of graph ordering requires the additional inequality.

Sometimes matrices $X$ fulfill Eq.3 without representing functions. A proper $X$ must be row stochastic, otherwise nodes could have multiple images. If $X$ were nevertheless column stochastic, the equation ought to be rearranged to take advantage of the implied inverse function.

The multiplicity of links often interferes with the interpretation of Eq. 3; to define homomorphism it is the pattern of zeroes which is relevant; matrix operations should be performed with boolean algebra followed by a numerical comparison, or else the nonzero elements should be normalized to ones before comparison. One is fortunate when ordinary algebra suffices for an entire calculation, which is the only way that additional conclusions regarding eigenvalues and eigenvectors will be valid.

### 4.3 Regular expression

Since regular expressions describe only paths through a diagram but not the nodes themselves, a homomorphism between regular expressions is a bit harder to describe. Probably one would convert any given expression to a diagram, map the diagram, then construct a new regular expression. As it is, unions form a part of the definition of regular expressions, but the computation of intersections and complements typically reverts to a diagram or a machine.

## 5 Dual diagrams

Just as links join pairs of nodes in a diagram, it can be said that nodes join pairs of links. If links were drawn as nodes and conversely, a new diagram, called the dual, could be established. Sometimes a dual is more concise than the original; and sometimes it just reveals its information in a more desirable form.

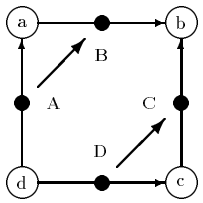



Figure 5: The dual of a diagram lets links be nodes.

## 5.1 The tail-head factorization

The matrix representation of a diagram can be factored into a product of matrices, generally rectangular, which relate the nodes and links to one another, rather than nodes to nodes or links to links. Using capital letters for links, small letters for nodes, the matrix elements of the factors are generally boolean propositions such as "node $a$ lies at the tip of link $B$." Then the node linking matrix is the product $\mathcal{L} = \mathcal{T}\mathcal{H}^T$,

$$\text{link}(i,j) = \sum_K \text{tail}(i,K)\text{head}^T(K,j),$$

whilst the link joining matrix is $\mathcal{N} = \mathcal{H}^T\mathcal{T}$, or

$$\text{node}(I,J) = \sum_k \text{head}^T(I,k)\text{tail(k, J)}.$$

Figure 5 shows a diagram upon which its dual has been superimposed; the $\mathcal{T}\mathcal{H}^T$ factorization for $\mathcal{L}$ is:

$$\begin{bmatrix} . & 1 & . & . \\ . & . & . & . \\ . & . & 1 & . \\ 1 & . & . & 1 \end{bmatrix} \begin{bmatrix} 1 & . & . & . \\ . & 1 & . & . \\ . & 1 & . & . \\ . & . & 1 & . \end{bmatrix} = \begin{bmatrix} . & 1 & . & . \\ . & . & . & . \\ . & 1 & . & . \\ 1 & . & 1 & . \end{bmatrix}.$$

Reversing the order of the factors produces $\mathcal{N}$:

$$\begin{bmatrix} 1 & . & . & . \\ . & 1 & . & . \\ . & 1 & . & . \\ . & . & 1 & . \end{bmatrix} \begin{bmatrix} . & 1 & . & . \\ . & . & . & . \\ . & . & 1 & . \\ 1 & . & . & 1 \end{bmatrix} = \begin{bmatrix} . & 1 & . & . \\ . & . & . & . \\ . & . & . & . \\ . & . & 1 & . \end{bmatrix}$$

There is a temptation to repeat the process to obtain a series of higher order duals; likewise one wonders about the reverse, whereby a given diagram could be exhibited as the dual of another.

## 5.2 Duals and homomorphism

The head matrix $\mathcal{H}$ is column stochastic, because only one node can be the head of a link; of course several links can terminate at the same node. Similarly the tail matrix $\mathcal{T}$ is row stochastic, there being only one tail to a given link. Strictly stochastic means that elements sum up to one, but the only possibility for integer elements in such a sum are zeroes and ones; just one single one may be present.

Dedicating the letters $R$ and $C$ to such matrices is more mnemonic than using $\mathcal{H}$ and $\mathcal{T}$; passing to the dual matrix $M^D$ then amounts to finding a CR factorization

$$M = CR, \tag{4}$$

then writing

$$M^D = RC. \tag{5}$$

The second dual would result from writing

$$RC = C_1 R_1 \tag{6}$$

with

$$M^{DD} = R_1 C_1, \tag{7}$$

and so on.

Note that if Equation 5 is multiplied on the right by $R$, the result

$$M^D R = RCR = RM, \tag{8}$$

asserts that $M^D$ is homomorphic to $M$. So also is the second dual (and all the rest, for that matter), inasmuch as

$$\begin{aligned} M^{DD}(R_1 R) &= (R_1 C_1) R_1 R \\ &= R_1 (C_1 R_1) R \\ &= R_1 (RC) R \\ &= (R_1 R) M. \end{aligned}$$

The matrix $R$ which generates the homomorphism from the dual to its graph associates each link with its terminal node.

## 5.3 The head-tail factorization

Going in the other direction, it would be nice to know when the $CR$ factorization is possible, independently of whether $RC$ was available for comparison or not.

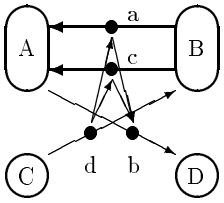



Figure 6: The antidual of a diagram lets nodes be links.

The rules of matrix multiplication are such that when $R$ is used as a left factor, it simply rearranges the rows of the left factor. Thus in any product $RA = N$, $A$ would have the same rows as $N$. But if $A$ were of type $C$, different rows would have to have their ones in different columns, a restriction which could be summarized by saying that the rows were orthogonal. Consequently the rows of $N$ would have to be either identical or orthogonal; lacking this characteristic it could not have an $RC$ factorization. Conversely, dual diagrams necessarily show the evidences of such a composition.

Given the necessary conditions, factors $R$ and $C$ can be constructed; a lack of uniqueness will be evident in some of the steps. To begin with, $C$ must have at least the distinct rows of $N$ (including a zero row if necessary) arranged in some order. But if $N$ has one or more columns of zeroes, some rows containing ones must be provided lest $C$ be nonstochastic.

The final number of rows chosen determines the number of columns of $R$, which is filled in at last by placing the rows of $C$ in their proper place in $N$. Zero rows in $N$ must be created by copying a row from $C$—not using zero coefficients in $R$—in order to keep $R$ stochastic.

If the diagram of Figure 5 is given this treatment, we find the antidual shown in Figure 6, calculated as follows:

$$\begin{bmatrix} 1 & . & . & . \\ . & . & . & 1 \\ 1 & . & . & . \\ . & 1 & . & . \end{bmatrix} \begin{bmatrix} . & 1 & . & . \\ 1 & . & 1 & . \\ . & . & . & 1 \\ . & . & . & . \end{bmatrix} = \begin{bmatrix} . & 1 & . & . \\ . & . & . & . \\ . & 1 & . & . \\ . & . & . & . \end{bmatrix};$$

reversing the order yields the graph to which it is dual:

$$\begin{bmatrix} . & 1 & . & . \\ 1 & . & 1 & . \\ . & . & . & 1 \\ . & . & . & . \end{bmatrix} \begin{bmatrix} 1 & . & . & . \\ . & . & . & 1 \\ 1 & . & . & . \\ . & 1 & . & 1 \end{bmatrix} = \begin{bmatrix} . & . & . & 1 \\ 2 & . & . & . \\ . & 1 & . & . \\ . & . & . & . \end{bmatrix}$$

Interestingly, this antidual contains a double link, whose importance is evident from Figure 6.

For a thorough presentation of duals, which they call "line graphs," Robert Hemminger and Lowell Beinecke's survey [5] should be consulted. Among other things they cite criteria which avoid the presence of self-loops and multiple links in the dual diagram. Essentially there is a list of configurations such as the example presented here, which have to be avoided. The dichotomy "identical or orthogonal" which figures in the construction of the antidual was formulated by Paul Richards [6] in 1967.

## 5.4 Counting paths

There is an interesting relation between the number of paths in a diagram and the number to be found in the dual diagram. Recall that the elements of powers of the connectivity matrix $M$ represent the number of paths joining the row index node to the column index node; if the respective sums are taken, the total number $n$ of paths results. In matrix form, taking $u$ to be a vector whose components are all ones,

$$n(M) \quad = \quad u^T M u. \tag{9}$$

Given that $u$ is an eigenvector (with unit eigenvalue) of a row stochastic matrix just as $u^T$ is a similar eigenvector of a column stochastic matrix, it follows from the $RC$ decomposition of the dual that

$$\begin{aligned} u^T M^2 u &= u^T RCRCu \\ &= u^T CRu \\ &= u^T M^D u \end{aligned}$$

Hence $n(M^2) = n(M^D)$; entirely similar reasoning reveals that

$$n(M^k) \quad = \quad n((M^D)^{k-1}) \tag{10}$$

Although the matrices figuring in the equation are not likely to be identical to their duals, they both contain the same number of 1's; in particular the number of paths of length 2 in any diagram is the same as the number of links in its dual diagram. Note that this is a property of *directed* graphs, not necessarily of general graphs.

Another useful property of duality is the relation between Hamiltonian paths and Eulerian paths. A Hamiltonian path is one which visits each node of the diagram once (clearly, the diagram must be connected), while an Eulerian path is one which traverses every link once (in the proper direction) even though nodes are repeated during the voyage. A Hamiltonian path, one of which is usually hard to find, becomes an Eulerian path in the antidual diagram, criteria for which are generally easier to obtain. The result would be more useful if more graphs actually had antiduals.

### 5.5 Eigenvalues and eigenvectors

A further consequence of equality in Eq. 3 is that except for a possible discrepancy associated with zero, the eigenvalues and eigenvectors of the connectivity matrix associated with a homomorphic image are the same as for the diagram itself. Suppose that $A$ and $B$ are the matrices and that $z$ is an eigenvector of $B$.

$$Bz = \lambda z.$$

Then

$$\begin{aligned} XBz &= AXz \\ &= \lambda Xz, \end{aligned}$$

making $Xz$ an eigenvector of $A$ with the same eigenvalue. A similar relation, valid in the opposite direction, holds for the row eigenvectors. Precaution is necessary when $\lambda$ vanishes, as it must when $A$ and $B$ have different dimensions; the numbers of eigenvectors associated with zero will differ.

## 6 Reverses and complements

Besides the chain of duals, there are other related graphs which can be derived from an originally given graph.

### 6.1 Reversed graph

The definition of a graph which we have employed is not the usual one to be found in the literature; technically our graphs are called *digraphs* (a contraction of "directed graph"). The reasons are historical, inasmuch as the concern with a graph was the linkages between is nodes which were originally conceived as a mutual connection between the two nodes involved.

From the point of view of an algebraic treatment of the connectivity matrix, symmetrical linkages are desirable because they lead to symmetrical matrices, for which there are much more convenient estimates of eigenvalues and procedures for obtaining the eigenvectors and eigenvalues.

On the other hand, actual eigenvalues (other than the largest and possibly the second largest) do not have much direct application to graphs, nor is the decomposition according to eigenvectors particularly relevant. Consequently there is little reason to insist upon symmetrical linkages, particularly given the existence of a very complete theory of positive (asymmetrical) matrices which does include the most useful aspects of eigenvalues and eigenvectors.

Applications to automata envisage directed links, just as the development given so far supposes, and certainly encompass the symmetrical case — just

include every link twice, once in each direction. A symmetrical graph is just a special case; every graph can be symmetrized by adjoining reverse links, and one can define the *reverse* of any graph $(N, L)$: merely reverse every link.

$$\begin{aligned} (N, L)^R &= (N, L^T) \\ L^T &= \{(x, y) \ni (y, x) \in L\} \end{aligned} \tag{11}$$

The connectivity matrix of a reversed graph is the transposed matrix, described by the reversed regular expression, in which each sequence is written backwards.

## 6.2 Complementary graph

There is sufficient occasion to mention that certain links are *not* in a graph that it is convenient to construct a new graph composed entirely and exclusively of the missing links. The result is the *complement* of the given graph.

$$\begin{aligned} (N, L)^C &= (N, \bar{L}) \\ \bar{L} &= \{(x, y) \ni (y, x) \notin L\} \end{aligned} \tag{12}$$

If it is not desired that all the links running in the wrong direction be included in the complement, the graph should be symmetrized before complementation.

At least when a graph contains single links without multiplicity, the connectivity matrix of the reversed graph is $A - U$, supposing that $A$ is the matrix of the original graph and that $U$ is a conformable square matrix, all of whose components are ones.

In terms of Eq. 3, for a homomorphism to preserve non-links (that is, the complementary graph) requires that

$$(U_1 - A)X \leq X(U_2 - B). \tag{13}$$

However, $XU_2 = U_x$ is a consequence of the definition of a function, that every point have one and only one image. Likewise $U_1 X \geq U_x$ holds when the function is *onto* and $X$ lacks a zero column; together

$$XU_2 \leq U_1 X. \tag{14}$$

The subscripts on $U$ remind us that the dimension of each of the matrices may be different. Subtracting Eq. 13 from Eq. 14 and reversing the equality to compensate the sign produces

$$AX \geq XB. \tag{15}$$

Comparison now yields the derivation of the assertion that equality in Eq. 3:

$$AX = XB. \tag{16}$$

corresponds to the preservation of both links and non-links; note that $X$ must be *onto* and not just *into* to get the result.

The strong homomorphism expressed in Eq. 16 guarantees that eigenvalues and eigenvectors of the image matrix belong to the source matrix as well: consider

$$BZ = \lambda Z \tag{17}$$
$$XBZ = \lambda XZ \tag{18}$$
$$A(XZ) = \lambda(XZ). \tag{19}$$

Similar relations, in the opposite direction, hold for eigenrows.

# 7 The de Bruijn diagram

It is nearly impossible to do any work with linear cellular automata without encountering the fact that their neighborhoods overlap, so that it is preferable to begin with this circumstance as a fundamental fact. Shift register theory is a discipline based on the treatment of overlapping sequences, so it is not surprising that its fundamental tool, the de Bruijn diagram, would be useful for automata theory.

Although this diagram is explained in Solomon Golomb's fundamental book [7] on shift registers, it actually has a venerable history which has been traced by Anthony Ralston in an article in the *American Mathematical Monthly* [8].

## 7.1 Definition

The nodes of the de Bruijn diagram are sequences of symbols from some alphabet, just as regular expressions are. They can even be sequences of nodes from a specific graph. The links of the diagram describe how such sequences may overlap. Different degrees of overlap lead to different diagrams, the simplest of which overlap according to the gain or loss of a single initial or terminal symbol. Thus the binary sequence 0011 overlaps the sequence 0110 by losing 0 as its initial symbol, whereas the second sequence overlaps through the loss of 0 as a terminal symbol. The link can be labelled according to the displaced symbol, as well as by the composite sequence 00110, and a variety of other ways. The intended application generally governs the choice.

When the symbols are consecutive integers they can be treated as elements of a ring or perhaps a finite field; the ease of discussing their properties arithmetically or algebraically makes the choice eminently worthwhile. For example,

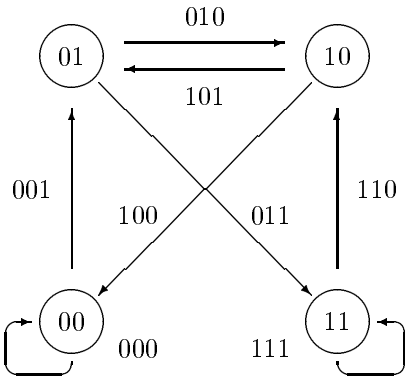



Figure 7: The generic (2,1) de Bruijn diagram.

the topological matrix of a de Bruijn diagram becomes simply

$$\begin{aligned} M_{ij} &= 1 \quad j = \begin{cases} ki \\ ki+1 \\ \cdots \\ ki+k-1 \end{cases} \pmod{k^{2r}} \\ &= 0 \quad \text{otherwise.} \end{aligned}$$

## 7.2 Subdiagrams

Through the intermediary of a de Bruijn diagram, graphs can represent configurations, or classes of configurations, in cellular automata. The links of a de Bruijn diagram are naturally associated with the neighborhoods of an automaton using the same symbols, which associates the links with a step of evolution in an equally natural fashion. If there is any reason to discriminate between neighborhoods, the same discrimination may define a subdiagrams of the de Bruijn diagram. A good example of the process arises from the still lifes—configurations of cells which do not change during the course of evolution.

The generic de Bruijn diagram for a (2,1) automaton (one having two states per cell with a single neighbor on each side, according to Stephen Wolfram's notation [9]) has four nodes corresponding to the four two-cell partial neighborhoods, with eight links representing the full three-cell neighborhoods. Such a diagram is shown in Figure 7.

The still life diagram may be extracted from the generic diagram by removing all links which do not conserve their central cell during the automaton's

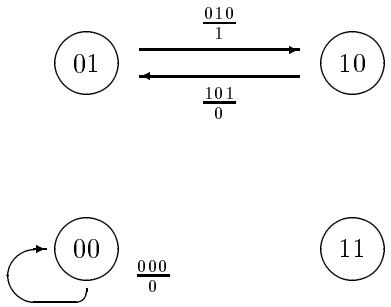



Figure 8: Subdiagram generated by Rule 22 still lifes.

evolution. Loops in the subdiagram composed of the remaining links define sequences, rather than individual cells, which are invariant to evolution. By reading off such sequences, all the still lifes for the automaton are automatically determined.

In general any boolean combination of the cells of the neighborhood and the evolved cell may determine the subdiagram, leading to chains of cells all of which fulfill the same property. As an example, one important binary automaton evolves according to the so-called Rule 22 [9]:

| neighborhood | 000 | 001 | 010 | 011 | 100 | 101 | 110 | 111 |
|---|---|---|---|---|---|---|---|---|
| image | 0 | 1 | 1 | 0 | 1 | 0 | 0 | 0 |

The de Bruijn diagram has eight links connecting four nodes (namely, 00, 01, 10, and 11); keep or reject the links according to whether they conserve their central cell, with results summarized by the following table:

| neighborhood | 000 | 001 | 010 | 011 | 100 | 101 | 110 | 111 |
|---|---|---|---|---|---|---|---|---|
| keep | yes | no | yes | no | yes | no | no | no |

Figure 8 shows the resulting subdiagram, which evidently consists of two disjoint loops; the first, of length 1, leads to an unending sequence of zeroes while the second, of length 2, leads to an alternating sequence of zeroes and ones. These are exactly the still life configurations for this rule.

There is an inverse application for Figure 8; suppose that it had beed decided beforehand that one needed a rule with quiescent zeroes and the combination $(01)^*$ as a still life. If so, the loops in the figure are forced, but the remaining five links can be assigned arbitrary values. All told there are thirty two rules with the required still lifes. To the extent that the required loops can be found, rules can be located which meet almost any desired specification.

### 7.3 A master diagram

Evidently the subdiagram consists of two disjoint loops; the first, of length 1, leads to an unending sequence of zeroes while the second, of length 2, leads to an alternating sequence of zeroes and ones. These are exactly the still life configurations for this rule.

Perhaps it is worth emphasizing the point that there are many diagrams which can be associated with a cellular automaton, a significantly large proportion of which are subdiagrams of a de Bruijn diagram. Many of the remainder are associated with extensions of de Bruijn diagrams; altogether de Bruijn diagrams constitute a central reference point in a context that might have seemed to be open to any arbitrary kind of diagram.

The literature of automata theory shows varying degrees of awareness of the diagram; much contains intuition that was never formalized, but as time passes references have become more centralized and specific. For example, there are treatments of automata in terms of formal language theory [10, 11] which refer to "regular expression diagrams," which are recognizable as subdiagrams of a de Bruijn diagram. Masakazu Nasu [12] refers to them by name and invokes their properties; Erica Jen [13] refers to them, and it is likely that a diligent search would turn up still further instances of their use.

By using longer neighborhoods, the results of more than one generation of evolution may be incorporated in the criterion defining the subdiagram. In that way arbitrary combinations of shifts and periodicities may be studied, not to mention even more elaborate combinations. The following list mentions some of the additional possibilities.

1. evolution to a constancy after $n$ generations.
2. evolution of the cells of binary automaton into their complements; permutation of the values of the cells of an arbitrary automaton.
3. a quiescent state is one which does not change when its entire neighborhood is quiescent; a nilpotent rule (of order $n$) is one for which all cells become quiescent after $n$ generations.
4. a configuration is idempotent (of order $n$) if, for the $n^{th}$ generation and thereafter, the values of its cells do not change. A rule is idempotent if all configurations are idempotent.
5. a configuration is superluminal if it shifts a distance greater than the radius of the neighborhoods in each generation.

## 8 The de Bruijn matrix

The topological matrix of a de Bruijn diagram is quite regular, although it is asymmetrical and differs from circulant matrices, tridiagonal matrices, or

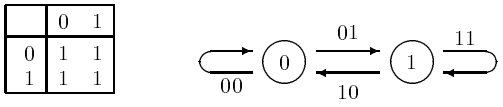



Figure 9: Single stage binary de Bruijn diagram.

other specialized forms which have been extensively analyzed in the literature. De Bruijn matrices $D_{k,s}$ or $D_s$ for short, are characterized by $k$, the number of symbols from which sequences may be formed, and $s$—the number of stages—which is the length of the sequence. In these terms, there will be $k$ links entering each node, as well as $k$ links leaving each node. In turn there will be $k^s$ nodes, with altogether $k^{(s+1)}$ links to join them, corresponding to sequences of length $s+1$.

The uniform distribution of the numbers of incoming and outgoing links means that the topological matrix has constant row sums as well as constant column sums; therefore divided by $k$ would be a doubly stochastic matrix with maximum eigenvalue 1 having a uniform probability distribution for its eigenvector.

It is worth presenting one or two examples and then the general case.

## 8.1 One stage binary matrix

A one stage de Bruijn diagram connects every node with every other node, making a full diagram with $k$ nodes and $k^2$ links. Its topological matrix is filled with 1's; a binary example is shown in Figure 9. The minimal equation satisfied by the binary matrix, $D_{2,1}^2 = 2U_{2,1}$, is a special case of the general equation $D_{k,1}^2 = kD_{k,1}$. Here and subsequently $U$ is a matrix all of whose elements are ones, just as $I$ will stand for the unit matrix.

## 8.2 Two stage binary matrix

Not every node of a two stage diagram or beyond links to all the other nodes; their topological matrices present the form of a series of staircases, corresponding to the diagram shown in Figure 7.

$$D_2 = \begin{bmatrix} 1 & 1 & . & . \\ . & . & 1 & 1 \\ 1 & 1 & . & . \\ . & . & 1 & 1 \end{bmatrix}$$

Simple calculation reveals that the minimal equation is $D^3 = 2D^2$ with eigenvalues 2, 0, 0, and principal vectors

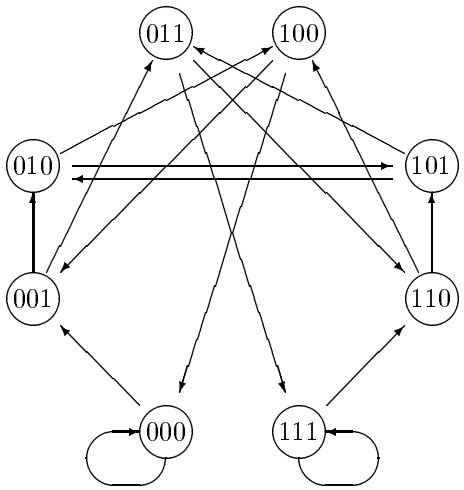



Figure 10: Generic (2,3/2) de Bruijn diagram.

$$R_2 = \begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & -1 & -1 & 1 \\ 1 & 1 & -1 & -1 \\ 1 & -1 & 1 & -1 \end{bmatrix}.$$

given that one of the zero eigenvalues has a $2 \times 2$ Jordan block.

## 8.3 Three stage binary matrix

By the third stage the staircase is fully evident; each step contains $k$ 1's, likewise there are $k$ staircases:

$$D_3 = \begin{bmatrix} 1 & 1 & . & . & . & . & . & . \\ . & . & 1 & 1 & . & . & . & . \\ . & . & . & . & 1 & 1 & . & . \\ . & . & . & . & . & . & 1 & 1 \\ 1 & 1 & . & . & . & . & . & . \\ . & . & 1 & 1 & . & . & . & . \\ . & . & . & . & 1 & 1 & . & . \\ . & . & . & . & . & . & 1 & 1 \end{bmatrix}$$

The minimal equation is readily determined to be $U^4 = 2U^3$, and as before the Jordan normal form prevails.

There are two interesting factorizations, both of which are quite general: $D_3 = P_3 U_3$ according to

$$D_3 = \begin{bmatrix} 1 & . & . & . & . & . & . & . & . \\ . & . & 1 & . & . & . & . & . & . \\ . & . & . & . & 1 & . & . & . & . \\ . & . & . & . & . & . & 1 & . & . \\ . & 1 & . & . & . & . & . & . & . \\ . & . & . & 1 & . & . & . & . & . \\ . & . & . & . & . & 1 & . & . & . \\ . & . & . & . & . & . & . & 1 & . \end{bmatrix} \times \begin{bmatrix} 1 & 1 & . & . & . & . & . & . & . \\ 1 & 1 & . & . & . & . & . & . & . \\ . & . & 1 & 1 & . & . & . & . & . \\ . & . & 1 & 1 & . & . & . & . & . \\ . & . & . & . & 1 & 1 & . & . & . \\ . & . & . & . & 1 & 1 & . & . & . \\ . & . & . & . & . & . & 1 & 1 & . \\ . & . & . & . & . & . & 1 & 1 & . \end{bmatrix}$$

and $D_3 = Q_3 U_3$ according to

$$D_3 = \begin{bmatrix} . & 1 & . & . & . & . & . & . & . \\ . & . & . & 1 & . & . & . & . & . \\ . & . & . & . & . & . & 1 & . & . \\ . & . & . & . & . & . & . & . & 1 \\ 1 & . & . & . & . & . & . & . & . \\ . & . & 1 & . & . & . & . & . & . \\ . & . & . & . & 1 & . & . & . & . \\ . & . & . & . & . & . & . & 1 & . \end{bmatrix} \times \begin{bmatrix} 1 & 1 & . & . & . & . & . & . & . \\ 1 & 1 & . & . & . & . & . & . & . \\ . & . & 1 & 1 & . & . & . & . & . \\ . & . & 1 & 1 & . & . & . & . & . \\ . & . & . & . & 1 & 1 & . & . & . \\ . & . & . & . & 1 & 1 & . & . & . \\ . & . & . & . & . & . & 1 & 1 & . \\ . & . & . & . & . & . & 1 & 1 & . \end{bmatrix}$$

Several relationships among these matrices are evident; for example:

$$\begin{aligned} D_n &= P_n(I_{n-1} \otimes D_1) \\ &= (D_1 \otimes I_{n-1})P_n \\ &= Q_n(I_{n-1} \otimes D_1) \\ &= (D_1 \otimes I_{n-1})Q_n \end{aligned}$$

wherein $I$ is the unit matrix. The factors satisfy several identities, of which the most useful are:

$$U_n^2 = 2U_n,$$

$$P_n + Q_n = D_n.$$

$P$ and $Q$ are noncommuting permutation matrices; nevertheless the noncommutative binomial theorem can still be used to evaluate powers of $D$. Whatever scheme is used, the essential observation is that powers of $D$ exhibit broader steps and more numerous ladders until the matrix is solidly filled with 1's; from then on successive powers merely differ by the factor $k$.

## 8.4 General de Bruijn matrix

Thus there are both factorizations and sum decompositions for the de Bruijn matrix, all readily obtained in a way that indicates many more representations are possible, none quite as symmetrical as the ones shown. For $k > 2$ there are

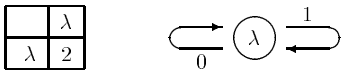



Figure 11: Zero stage binary de Bruijn diagram.

additional permutation matrices which participate in the decompositions, and the blocks in the matrix $U$ are correspondingly larger. The factored forms show that the determinant of any de Bruijn matrix is zero, but it is not difficult to obtain the entire minimal equation, which is

$$D_{k,n}^{n+1} = kD_{k,n}^{n}, \tag{20}$$

nor is it difficult to verify that

$$Tr(D_{k,n}^{n}) = k^n \tag{21}$$

for all values of $n$. This is the count of loops of length $n$, wherein each loop is weighted by the number of nodes it contains. It must be borne in mind that *all* loops are counted, including the degenerate cases where the same cycle of nodes is traversed several times.

## 8.5 RC and CR factorizations

Bearing in mind the relation between a diagram and its dual established in Section 5.2, it is not surprising to see that all the de Bruijn diagrams for $k$ states form a chain of duals. In fact, $D_0$, the null string occupying its single node (see Figure 11), could begin the chain.

In any event we can start the chain with

$$\begin{aligned}
2 &= D_0 \\
D_0 &= \begin{bmatrix} 1 & 1 \end{bmatrix} \begin{bmatrix} 1 \\ 1 \end{bmatrix} \\
\begin{bmatrix} 1 \\ 1 \end{bmatrix} \begin{bmatrix} 1 & 1 \end{bmatrix} &= \begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix} (= D_1) \\
D_1 &= \begin{bmatrix} 1 & 1 & . & . \\ . & . & 1 & 1 \end{bmatrix} \begin{bmatrix} 1 & . \\ . & 1 \\ 1 & . \\ . & 1 \end{bmatrix} \\
\begin{bmatrix} 1 & . \\ . & 1 \\ 1 & . \\ . & 1 \end{bmatrix} \begin{bmatrix} 1 & 1 & . & . \\ . & . & 1 & 1 \end{bmatrix} &= \begin{bmatrix} 1 & 1 & . & . \\ . & . & 1 & 1 \\ 1 & 1 & . & . \\ . & . & 1 & 1 \end{bmatrix} (= D2)
\end{aligned}$$

$$D_2 = \begin{bmatrix} 1&1&.&.&.&.&.&. \\ .&.&1&1&.&.&.&. \\ .&.&.&.&1&1&.&. \\ .&.&.&.&.&.&1&1 \end{bmatrix} \begin{bmatrix} 1&.&.&. \\ .&1&.&. \\ .&.&1&. \\ .&.&.&1 \\ 1&.&.&. \\ .&1&.&. \\ .&.&1&. \\ .&.&.&1 \end{bmatrix}$$

wherein the pattern of the factorization is fairly evident. Suppose that $I_n$ is a $k^n \times k^n$ unit matrix and that $u$ is a $k$-dimensional vector with unit components. Then evidently

$$\begin{aligned} (u \otimes I_n)(I_n \otimes u^T) &= D_{n+1} \\ D_n &= (I_n \otimes u^T)(u \otimes I_n) \end{aligned}$$

From this it is immediately clear that the whole chain of binary de Bruijn matrices has the single nonzero eigenvalue $k$ belonging to $D_0$. Note that the factors in the Kronecker product cannot be multiplied together because they are not conformable; the formulas stand as written.

## 8.6 Hamiltonian and Eulerian paths

Hamiltonian paths in a diagram are those which visit each vertex once and only once; Hamiltonian loops are those for which the tour returns to the starting point. In contrast Eulerian paths are those which use every edge in the diagram once and only once, loops likewise completing a circuit by returning to the start.

An Eulerian problem, to decide whether such paths exist or not, is readily soluble; for loops, each vertex must have as many incoming as outgoing links, and the diagram as a whole must be connected (which is certainly true of a de Bruijn diagram). For paths, the terminal nodes could be separated, allowing one extra outgoing link at the initial node plus a surplus incoming link at the terminal node. Euler's classical result refers to undirected links; I. J. Good [14] proved the analogous directed variant in 1946.

A Hamiltonian problem is usually intractable, but for de Bruijn diagrams, the dual of a diagram of $n$ stages is the diagram of $n+1$ stages. Consequently, running through all the links in any diagram is equivalent to running through all the nodes of its successor, allowing the Eulerian result to solve the equivalent Hamiltonian problem for an additional stage.

Demonstrating existence is much easier than counting, in turn simpler than exhibiting, paths. In 1946 N. J. de Bruijn [15] obtained a recursion relation to count the Hamiltonian paths in a binary diagram exploiting duality, which he called *doubling*; a sufficiently significant result to associate his name with the

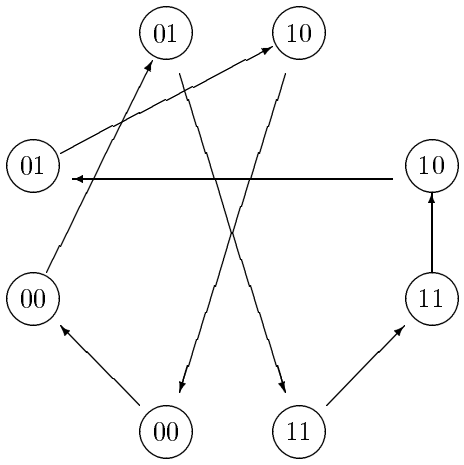



Figure 12: A Hamiltonian path in the (2,3/2) de Bruijn diagram.

graph. Additional discussion can be found in Marshall Hall, Jr.,'s *Combinatorial Theory* [16].

When diagrams are both Hamiltonian and Eulerian, every Hamiltonian circuit can be promoted to an Eulerian circuit and the interesting question is to determine in how many ways. Shift register theory esteems the actual sequences highly; a good part of Golomb's book [7] concentrates on obtaining them. Automata theory is less concerned with this particular detail, but it is still useful to know some procedures.

An upper bound on the number of Hamiltonian cycles is always that number of cycles whose length matches the number of nodes. Since the diagram of order $n$ has $k^n$ nodes, by Eq. 21 this number is $k^{k^n}$. For binary diagrams, de Bruijn's value is $2^{2^{n-1}-n}$. Aside from number theoretic deformations at low values of $n$, comparison of the results would lead one to believe that $(1/k)^{th}$ of all candidates are Hamiltonian.

Similarly, the number of loops whose length equals the total number of links bounds the number of Eulerian cycles; in both cases, degenerate loops must be discounted to get the true count.

Figure 12 illustrates several of the points which have been discussed; it shows one of the two Hamiltonian paths associated with the matrix $D_3$, but the nodes have been labelled according to $D_2$. Homomorphism is apparent—the numerical node indices have been reduced modulo 4, while the residues modulo 2 (linkages) have not changed. If duplicate nodes were superimposed and reference made

to Figure 7, one of the Eulerian loops of the latter would manifest itself; a Hamiltonian path wrapped around the image twice.

There is an embedment in the opposite direction too—the $(2, 1)$ diagram fits into just half of the $(2, 3/2)$ diagram. All the arrows are there; homomorphism fails when they don't all close up within the image of $(2, 1)$ itself, the trick is to match up two copies of the image to get the next diagram. In fact, when this arrangement presents itself one should always try to arrange an inverse homomorphism.

# 9 Subset diagrams

So far no great importance has been attached to labelling the links in a graph, although it is clearly possible to do so. But often labelled links are supposed to belong to different classes, implying that the links should be distinguished accordingly. In turn the classes would have individual connectivity matrices. Instead of just tracing paths through the diagram, it could be required that the labels follow a certain sequence, with the attendant question of whether the required path actually exists; a question that could be resolved by multiplying the corresponding connectivity matrices in the prescribed order.

Frequently the question is more general — does the required path exist anywhere at all in the diagram? One approach would be to list all the paths, so as to search the list for the presence of the candidate. Something of the nature can hardly be avoided, so it is a matter of organizing the technique, which is usually known as Moore's subset construction [17], which was introduced in 1956 by Edward F. Moore for a different reason.

## 9.1 Scalar subset diagram

The nodes are grouped into subsets, note being taken of the subsets to which one can arrive through systematic departures from all the nodes in any given subset. The result is a new graph, with subsets for nodes and links summarizing all the places that one can get to from all the different combinations of starting points. Sometimes, but far from always, the possible destinations narrow down as one goes along; in any event one has all the possibilities cataloged.

One point to be observed is that if one thinks that there should be a link at a certain node and there is not, the link should be drawn to the empty set instead; a convention which assures every label of having a representation at every node in the subset diagram.

Let $a$ and $b$ be nodes in a given diagram, $S$ a subset, and $|S|$ the cardinality

of $S$; then the formal definition of its subset diagram is

$$\Sigma_i(S) \quad = \quad \begin{cases} \phi & S = \phi \\ \{b \mid \mathrm{link}_i(a,b)\} & S = \{a\} \\ \bigcup_{a \in S} \Sigma_i(a) & |S| > 1 \end{cases} . \tag{22}$$

There is another important reason for working with subsets. Labelled links resemble functions, by associating things with one another. But if two links with the same label emerge from a single vertex, they can hardly represent a function. Forging the subset of all destinations, leaves one single link between subsets, bringing functionality to the subset diagram even though it did not exist originally. Including the null set ensures that every point has an image, avoiding partially defined functions.

Once the subset diagram has been formed, if a path leads from the universal set to the empty set, that is conclusive evidence that such a path exists nowhere in the original diagram. Another application—the one originally envisioned by Moore—is to determine whether there are paths leading to the unit classes. Such a paths, if they existed, could be used to force an automaton into a predetermined state, no matter what its original condition.

## 9.2 Vector subset diagram

Moore's traditional discussion gives no internal structure to the nodes of the subset diagram, but we will find it convenient to regard each node as a vector whose components are indexed by the nodes of the original graph. Then links in the subset graph are represented by projections applied to the topological matrix of the original graph; precisely, projection onto the subset belonging to the label in question. Each row of the graph will have $k$ nonzero submatrices (if that is the number of labels) except that if there is no link corresponding to some particular label, its submatrix will be zero too.

The column containing the submatrix for label $k$ will correspond to the subset of nodes which are destinations for that label. Should the destination subsets coincide for two or more labels, neither common nor impossible, the multiplicity should be entered into the submatrix. Alternatively, one could separate the subset matrices for each link and later sum them as needed.

If there were $n$ nodes in the original graph, the topological matrix of the subset diagram will have dimension $2^n \times 2^n$. For a g-stage de Bruijn diagram, $n = 2^g$. As usual, powers of the topological matrix describe chains with multiple links, but the most interesting matrix elements will be the ones in the top row, so to speak. They connect the full set with other subsets, including the empty set. If it is immaterial where a path begins or ends, the submatrix connecting the full set with itself suffices. Restrictions placed upon the choices of initial and terminal nodes will lead to other submatrices.

Were it not for the projections, the vector connection matrix $V$ would be the tensor product of the de Bruijn matrix with the scalar connection matrix. But the projected elements are missing; so introduce row and column indices of the form $(\sigma, m)$, where $\sigma$, $\tau$ are subsets whose own linkage is defined by

$$\text{Link}(\sigma,\tau) \quad = \quad \begin{cases} 1 & \tau = \text{link}^{-1}(\sigma) \\ 0 & \text{otherwise} \end{cases} \quad . \tag{23}$$

Then,

$$V_{\sigma m,\tau n} \quad = \quad \text{Link}(\sigma,\tau)\text{link}(m,n) \tag{24}$$

## 9.3 Rule 126

To illustrate the use of the subset diagram, consider the automaton for $(2,1)$ Rule 126:

| neighborhood | 000 | 001 | 010 | 011 | 100 | 101 | 110 | 111 |
|---|---|---|---|---|---|---|---|---|
| image | 0 | 1 | 1 | 1 | 1 | 1 | 1 | 0 |

In other words, all neighborhoods evolve into ones with the exception of 111 and the quiescent neighborhood 000, which evolve into zeroes. The de Bruijn diagram for this rule is $D_{2,2}$, which has the symbolic variant (dots represent the null word $\phi$):

$$\begin{bmatrix} 0 & 1 & . & . \\ . & . & 1 & 1 \\ 1 & 1 & . & . \\ . & . & 1 & 0 \end{bmatrix} = \begin{bmatrix} 0 & . & . & . \\ . & . & . & . \\ . & . & . & . \\ . & . & . & 0 \end{bmatrix} + \begin{bmatrix} . & 1 & . & . \\ . & . & 1 & 1 \\ 1 & 1 & . & . \\ . & . & 1 & . \end{bmatrix} .$$

Since the nodes $A = 00$, $C = 01$, $D = 10$, and $F = 11$ are linked by the symbols 0 and 1, the subset diagram can be constructed. It actually has $2^4$ nodes for the sixteen subsets, but to save space we show only the part connected to the full subset ($\phi$ is the empty set). First, note the destination of each arrow leaving individual nodes:

| node | 0 leads to | 1 leads to |
|---|---|---|
| $A$ | $A$ | $C$ |
| $C$ | $\phi$ | $D, F$ |
| $D$ | $\phi$ | $A, C$ |
| $F$ | $F$ | $D$ |

.

Then, form vectors whose elements are the tail nodes and whose components are indexed by the head nodes; an element is null if there is no incoming link

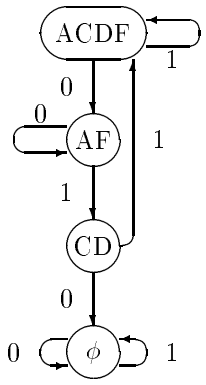



Figure 13: Subset diagram for Rule 126.

from any node.

| subset | 0 leads to | 1 leads to |
|---|---|---|
| $\{ACDF\}$ | $(A, \phi, \phi, F)$ | $(D, A+D, C+F, C)$ |
| $\{AF\}$ | $(A, \phi, \phi, F)$ | $(\phi, A, F, \phi)$ |
| $\{CD\}$ | $(\phi, \phi, \phi, \phi)$ | $(D, D, C, C)$ |
| $\{\}$ | $(\phi, \phi, \phi, \phi)$ | $(\phi, \phi, \phi, \phi)$ |

This structure is actually the vector subset diagram; the scalar subset diagram arises by enumerating the non-null indices (we don't care how many incoming arrows there are nor where they originate, as long as there is at least one):

| subset | 0 leads to | 1 leads to |
|---|---|---|
| $\{ACDF\}$ | $\{AF\}$ | $\{ACDF\}$ |
| $\{AF\}$ | $\{AF\}$ | $\{CD\}$ |
| $\{CD\}$ | $\{\}$ | $\{ACDF\}$ |
| $\{\}$ | $\{\}$ | $\{\}$ |

;

its topological matrix, having indexed the subsets in the order shown, is $S = a+b$ according to

$$\begin{bmatrix} 1 & 1 & . & . \\ . & 1 & 1 & . \\ 1 & . & . & 1 \\ . & . & . & 2 \end{bmatrix} = \begin{bmatrix} . & 1 & . & . \\ . & 1 & . & . \\ . & . & . & 1 \\ . & . & . & 1 \end{bmatrix} + \begin{bmatrix} 1 & . & . & . \\ . & . & 1 & . \\ 1 & . & . & . \\ . & . & . & 1 \end{bmatrix}.$$

The matrix is upper triangular, because the null set is linked only to itself. Only the $3 \times 3$ submatrix in the upper left hand corner is really necessary. The 2 in the lower right corner is not strictly required, attesting only to the fact

that *no* path from the null set has anywhere else to go, thereby conserving the uniform row sum.

Finally, the topological matrix of the vector subset diagram is

$$V = \left[\begin{array}{cccc|cccc|cccc}
. & 1 & . & . & 1 & . & . & . & . & . & . & . \\
. & . & 1 & 1 & . & . & . & . & . & . & . & . \\
1 & 1 & . & . & . & . & . & . & . & . & . & . \\
. & . & 1 & . & . & . & . & 1 & . & . & . & . \\
\hline
. & . & . & . & 1 & . & . & . & . & 1 & . & . \\
. & . & . & . & . & . & . & . & . & . & . & . \\
. & . & . & . & . & . & . & . & . & . & . & . \\
. & . & . & . & . & . & . & 1 & . & . & 1 & . \\
\hline
. & . & . & . & . & . & . & . & . & . & . & . \\
. & . & 1 & 1 & . & . & . & . & . & . & . & . \\
1 & 1 & . & . & . & . & . & . & . & . & . & . \\
. & . & . & . & . & . & . & . & . & . & . & .
\end{array}\right].$$

## 9.4 Structural observations

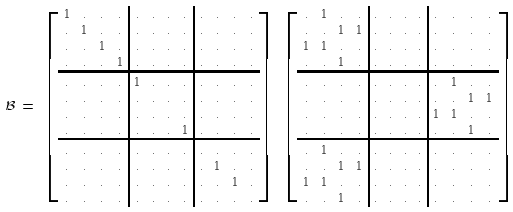
The topological matrix of the vector subset diagram manifests some interesting structural details. It is not quite a tensor product, but the nonzero submatrices fall exactly on the locations of the nonzero elements of the scalar matrix. The submatrices are of two types, corresponding to the decomposition of the symbolic de Bruijn matrix, being derived from them through multiplication on the right by a projection onto the subset defining the row. In the matrix shown, the projector for the first row is the identity matrix, for the second it preserves components $D$ and $F$, while the third goes with $A$ and $C$.

Moreover a supermatrix whose diagonal submatrices are the appropriate projectors commutes with the vector subset matrix, just as it commutes with each of the two summands resulting from the symbolic decomposition of the de Bruijn matrix. Incorporation of this projector as a factor allows writing the vector matrix as a sum of two tensor products, which in turn facilitates the evaluation of powers of the vector matrix and products of its summands.

Suppose that $S$ is the scalar subset matrix, $\Pi$ the projector, $V = \Pi\mathcal{V}$ the vector subset matrix, and that the de Bruijn matrix $D$ is decomposed into the sum $A + B$ according to a criterion such as the value of the evolved cell. Then we would have

$$\begin{aligned} V &= \mathcal{A} + \mathcal{B}, \\ \mathcal{A} &= \Pi(A \otimes a), \\ \mathcal{B} &= \Pi(B \otimes b); \end{aligned}$$

for example the factorization below defines $\mathcal{B}$:



An immediate consequence of this representation is the fact that in any product of supermatrices, all the submatrices are formed from products of the two terms into which the de Bruijn matrix is decomposed, even though they may eventually have to be projected to obtain a final result. This establishes a formal relation between the methods of this section and the procedures of Erica Jen [13] or Backhouse and Carré [4].

# 10 Use of the subset diagrams

An excellent application of the subset construction to linear cellular automata is to the search for the Garden of Eden—configurations which cannot evolve from any predecessor. The problem has two settings—for finite or periodically closed automata in which it is trivial due to finiteness, and for infinite automata. Later, the problem can be generalized to counting the counterimages, calculating the frequency distribution of the multiplicity of counterimages, and establishing the relationship between singlevaluedness and invertibility.

## 10.1 Garden of Eden

To apply the subset diagram to the construction of counterimages, begin with the de Bruijn diagram whose links are the neighborhoods of the automaton. The nodes would be partial neighborhoods whose overlap is attested by the links, and the links can be labelled by the value of the cell which evolves from them. This is a new labelling, different from that obtained from the cell by which the neighborhood is extended. For the latter, all the outgoing nodes have distinct labels, but not for the former unless that is the nature of the rule. Possible ambiguities will be resolved in the subset diagram. Starting from the universal node, following the path dictated by the new configuration, it is possible to obtain all the ancestral configurations.

For example, using Rule 126 and the diagram of the last section, the chain 010 leads form $\{ACDF\}$ to $\{AF\}$ to $\{CD\}$ to $\{\}$, the null set. Therefore there is no way that 010 can be part of any evolved configuration. On the other hand a sequence of 0's leads repeatedly to the subset $\{AF\}$, so there are always counterimages of $0^*$, the quiescent configuration.

Since the universal subset is the starting point, the counterimage might conceivably begin with any pair of states, but since $C$ and $D$ are missing from the repeating subset, there is no ancestor which terminates with either 01 or 10, a mixed pair of states. Such restrictions can prejudice the evolution of finite or cyclical chains of states, yielding additional ancestorless configurations that would not occur for infinite automata.

Moreover, if the infinite automaton is to be "quiescent at infinity," by having only a finite number of excited states, it may turn out that a similar ancestor is impossible.

Altogether, the principal value of the scalar subset diagram is to establish such things as

1. the shortest excluded words, the occurrence of any one of which creates a Garden of Eden configuration,

2. a maximum length for a minimal excluded word, which is the number of nodes in the portion of the subset diagram connected to the full subset,

3. whether exclusion occurs in stages, as key segments are built up.

4. a regular expression describing excluded words.

## 10.2 Counting counterimages

A vector subset diagram whose links have been labelled according to the evolution of an automaton allows the gathering of fairly subtle information. Its powers classify the counterimages they are counting *exactly* by initial and terminal partial neighborhoods, in addition to lumping them into subsets as the scalar matrix does.

Often this is a more elaborate classification than is needed; what really count are the de Bruijn fragments comprising the submatrices, classifying ancestors according to their initial and final partial neighborhoods. Generally further sorting by subsets of partial neighborhoods only serves to identify and count the Garden of Eden configurations quickly.

For example, continuing to use the example from Rule 126, the de Bruijn product for the sequence $0^*$ is

$$\begin{bmatrix} 1 & . & . & . \\ . & . & . & . \\ . & . & . & . \\ . & . & . & 1 \end{bmatrix}^n = \begin{bmatrix} 1 & . & . & . \\ . & . & . & . \\ . & . & . & . \\ . & . & . & 1 \end{bmatrix}.$$

which makes it clear that an infinite quiescent configuration has exactly two ancestors, itself and $1^*$; in any event, 01 and 10 are excluded both as initial sequences and as final sequences from finite configurations such as on a ring. Of course, this information can also be elicited from the scalar subset matrix by looking at all the paths originating from unit classes.

Counterimages can be counted three ways: quiescent at infinity, cyclic, or completely general. Let $\Pi$ be a typical product of de Bruijn fragments generating the counterimages of a configuration; then

$$t = [\Pi]_{q,q} = Tr(\pi_q \Pi), \tag{25}$$

where $q$ is the completely quiescent partial neighborhood, yields the number of counterimages quiescent at infinity. The single nonzero element of the projection operator $\pi_q$ occupies the $q$th position on the diagonal; the trace formulation provides a uniformity of treatment for all three cases.

For a cyclic automaton, it is appropriate to recognize that a cycle must begin and end on the same partial neighborhood by calculating (for unit matrix $I$)

$$t = Tr(\Pi) = Tr(I\Pi). \tag{26}$$

Finally, the appropriate unrestricted formula would be

$$t = u^T \Pi u = Tr(U\Pi), \tag{27}$$

where $u$ is a vector, $U$ a matrix, solidly filled with 1's. In fact, all three counts can be described by either a trace or an inner product, both of which are linear functionals for matrices.

Taking into account all possible products representing ancestors of a configuration of length $n$ requires evaluating

$$\alpha_1 = k^{-n} Tr(U(a+b)^n), \tag{28}$$

but $a+b = D$, the de Bruijn matrix which satisfies $DU = kU$ and $D^{k+r} = k^r D^k$. Altogether, then,

$$\alpha_1 = k^2. \tag{29}$$

The unsurprising average of ancestors per configuration being $k^2$, whenever some configuration has fewer, another must have more. When the imbalance is sufficiently severe, Garden of Eden configurations are required to compensate the configurations with multiple ancestors—a trivial result for finite automata but with interesting consequences for infinite automata.

The second and higher moments of the distribution of counterimages can be obtained from some additional matrix algebra. In the following sequence of substitutions, let $P$ be one of the $k^n$ (noncommuting) factors in the expansion of $D^n = (a+b)^n$.

$$\begin{aligned}
\alpha_2 &= k^{-n} \sum (Tr(UP))^2 \\
&= k^{-n} \sum Tr(UP \otimes UP) \\
&= k^{-n} \sum Tr((U \otimes U)(P \otimes P)) \\
&= k^{-n} Tr((U \otimes U) \sum P \otimes P) \\
&= k^{-n} Tr((U \otimes U)(a \otimes a + b \otimes b)^n)
\end{aligned}$$

If $\rho$ is the dominant eigenvalue of $a \otimes a + b \otimes b$, a term proportional to $\rho^n$ will result for large $n$.

Higher moments will depend on higher tensor powers of $a$ and $b$, while the same formula persists with a suitably subscripted $\rho$ and $\alpha$; for example

$$\begin{aligned} \alpha_3 &= k^{-n} Tr((U \otimes U \otimes U) \times \\ &\quad (a \otimes a \otimes a + b \otimes b \otimes b). \end{aligned} \tag{30}$$

In another direction, if the connectivity matrix had been decomposed into three classes of links $a$, $b$, and $c$, the second moment would have taken the form

$$\begin{aligned} \alpha_2 &= k^{-n} Tr((U \otimes U) \times \\ &\quad (a \otimes a + b \otimes b + c \otimes c)^n). \end{aligned} \tag{31}$$

# 11 Pair diagram

The cartesian product of graphs has many applications. As the upper bound of two graphs, it compares paths between two different diagrams (or two paths in the same diagram). It also appears in second moment (and therefore variance) calculation of path frequencies. As an example, Figure 14 shows the pair diagram (cartesian product of a graph with itself) for the $(2,1)$ de Bruijn diagram of Figure 7.

Its connectivity matrix is

$$P = \left[\begin{array}{cccc|cccc|cccc|cccc} 1&1&.&.&1&1&.&.&.&.&.&.&.&.&.&. \\ .&.&1&1&.&.&1&1&.&.&.&.&.&.&.&. \\ 1&1&.&.&1&1&.&.&.&.&.&.&.&.&.&. \\ .&.&1&1&.&.&1&1&.&.&.&.&.&.&.&. \\ \hline .&.&.&.&.&.&.&.&1&1&.&.&1&1&.&. \\ .&.&.&.&.&.&.&.&.&.&1&1&.&.&1&1 \\ .&.&.&.&.&.&.&.&1&1&.&.&1&1&.&. \\ .&.&.&.&.&.&.&.&.&.&1&1&.&.&1&1 \\ \hline 1&1&.&.&1&1&.&.&.&.&.&.&.&.&.&. \\ .&.&1&1&.&.&1&1&.&.&.&.&.&.&.&. \\ 1&1&.&.&1&1&.&.&.&.&.&.&.&.&.&. \\ .&.&1&1&.&.&1&1&.&.&.&.&.&.&.&. \\ \hline .&.&.&.&.&.&.&.&1&1&.&.&1&1&.&. \\ .&.&.&.&.&.&.&.&.&.&1&1&.&.&1&1 \\ .&.&.&.&.&.&.&.&1&1&.&.&1&1&.&. \\ .&.&.&.&.&.&.&.&.&.&1&1&.&.&1&1 \end{array}\right],$$

whose tensor product form is clearly visible.

It is not always necessary to distinguish between the members of a pair; the arrows in a graph require links to be defined as ordered pairs of nodes, but that does not necessarily require that a pair of links be taken in any particular order, for example.

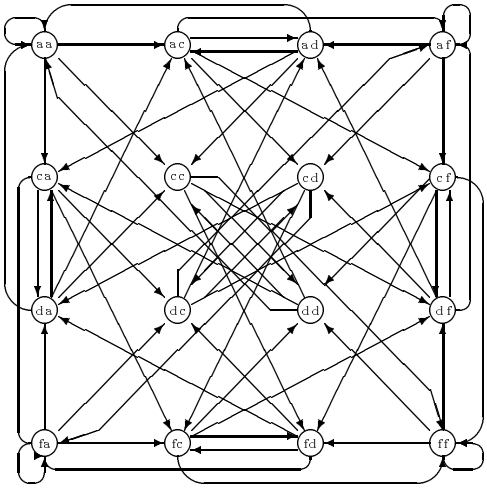



Figure 14: Sixteen node pair diagram for a $(2,1)$ de Bruijn diagram, an image of which is visible along the diagonal as well as in horizontal and vertical section.

Figure 15 shows the unordered pair graph of the two-stage de Bruijn diagram for $(2,1)$ automata, whose connectivity matrix is the symmetrized Kronecker product of the individual connectivity matrices. It has fewer nodes, yet the full Kronecker product is homomorphic to it, giving it computational and visual advantages.

Both versions satisfy Richard's criterion [6] for duality, presumably participating in the same kind of dual chains as the de Bruijn diagrams themselves.

The connectivity matrix for unordered pairs is

$$p = \begin{bmatrix} 1 & 1 & . & . & 1 & . & . & . & . & . \\ . & . & 1 & 1 & . & 1 & 1 & . & . & . \\ 1 & 1 & . & . & 1 & . & . & . & . & . \\ . & . & 1 & 1 & . & 1 & 1 & . & . & . \\ . & . & . & . & . & . & . & 1 & 1 & 1 \\ . & . & 1 & 1 & . & 1 & 1 & . & . & . \\ . & . & . & . & . & . & . & 1 & 1 & 1 \\ 1 & 1 & . & . & 1 & . & . & . & . & . \\ . & . & 1 & 1 & . & 1 & 1 & . & . & . \\ . & . & . & . & . & . & . & 1 & 1 & 1 \end{bmatrix},$$

while the homomorphism matrix between the two versions is

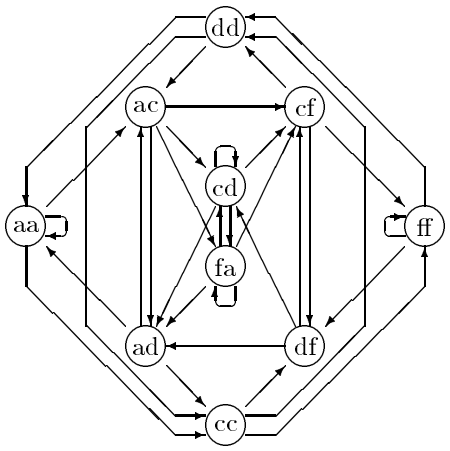



Figure 15: Ten node unordered pair diagram for a $(2,1)$ de Bruijn diagram, an image of which (the diagonal) is visible around the circumference.

$$X = \begin{bmatrix} 1 & & & & & & & & & \\ & 1 & & & & & & & & \\ & & 1 & & & & & & & \\ & & & 1 & & & & & & \\ & & 1 & & & & & & & \\ & & & & & 1 & & & & \\ & & & & & & 1 & & & \\ & & & & & & & 1 & & \\ & & 1 & & & & & & & \\ & & & & & & & & 1 & \\ & & & & & & & & & 1 \\ & & & & 1 & & & & & \\ & & & & & & & 1 & & \\ & & & & & & & & 1 & \\ & & & & & & & & & 1 \end{bmatrix}.$$

Multiplicities spoil comparing $PX$ to $Xp$:

$$\begin{bmatrix} 1&2&&&1&&&&&\\ &&1&1&&1&1&&&\\ 1&2&&&1&&&&&\\ &&1&1&&1&1&&&\\ &&1&1&&1&1&&&\\ &&&&&&&1&2&1\\ &&1&1&&1&1&&&\\ &&&&&&&1&2&1\\ 1&2&&&1&&&&&\\ &&1&1&&1&1&&&\\ 1&2&&&1&&&&&\\ &&1&1&&1&1&&&\\ &&1&1&&1&1&&&\\ &&&&&&&1&2&1\\ &&1&1&&1&1&&&\\ &&&&&&&1&2&1 \end{bmatrix} \neq \begin{bmatrix} 1&1&&&1&&&&&\\ &&1&1&&1&1&&&\\ 1&1&&&1&&&&&\\ &&1&1&&1&1&&&\\ &&1&1&&1&1&&&\\ &&&&&&&1&1&1\\ &&1&1&&1&1&&&\\ &&&&&&&1&1&1\\ 1&1&&&1&&&&&\\ &&1&1&&1&1&&&\\ 1&1&&&1&&&&&\\ &&1&1&&1&1&&&\\ &&1&1&&1&1&&&\\ &&&&&&&1&1&1\\ &&1&1&&1&1&&&\\ &&&&&&&1&1&1 \end{bmatrix}$$

But the discussion surrounding Equations 3 and 16, gives a choice: 1) reduce $PX$ to a boolean matrix whose nonzero entries are ones, or 2) weight the links in $p$ with the number of links per pair to get a numerically valid comparison.

# 12 Probabilistic de Bruijn matrix

The topological matrix of a de Bruijn diagram defines the connectivity of a diagram by indicating the different branches that arise when symbols are added and deleted from a sequence, but it takes no account of the likelihood that one or the other of the symbols will be chosen. If probabilities are incorporated in the matrix elements, it is just as easy to calculate the probability that a long string will occur as to establish the possibility of its presence in the first place.

## 12.1 Positive matrices

There is an extensive lore regarding the properties of positive matrices, dating from the work of Frobenius and Perron at the beginning of the century, and ably summarized in several contemporary textbooks, such as *Matrix Iterative Analysis* by Varga [18], *Non-Negative Matrices* by Seneta [19], and *Nonnegative Matrices in the Mathematical Sciences* by Berman and Plemmons [20]. A recent addition to this series is Minc's *Nonnegative Matrices*.

Applied to topological matrices, the theory yields estimates for such things as the increase in the numbers of paths through a network as the path length increases. Applied to probabilistic matrices it allows the determination of equilibrium configurations and the rapidity of approach to equilibrium from arbitrary initial configurations.

It is not surprising that the theory of positive matrices has strong applications to Markov chains and similar probabilistic concepts, or even that much of the motivation for their study came from this direction.

## 12.2 Largest eigenvalue

Gerschgorin estimates are somewhat easier to work with for positive matrices. Either of the two forms may be used

1. all eigenvalues lie within disks centered at the origin, whose radii are either the different row sums, or the different column sums. Whichever of the two yields the more restrictive results may be chosen.

2. all the eigenvalues lie within disks centered at the diagonal matrix elements, whose radii are the sums of the remaining elements in the respective row or column. Again, the more restrictive result may be used.

For positive matrices the additional information is available that the maximum eigenvalue must surpass the minimum row sum as well as being unable to reach the maximum row sum. Indeed the actual value is bounded away from these limits unless they coincide, there being results of various degrees of complexity for the actual bounds. The situation is described in Varga's book [18], along with references to original papers.

When working with a stochastic matrix, it is already a foregone conclusion that the maximum eigenvalue is 1.0, but the estimates are still valuable for non-stochastic matrices. The equilibrium eigenvector as well as the maximum eigenvalue can often be found by the expedient of successively squaring the matrix.

## 12.3 Second eigenvalue and convergence

For strictly positive matrices the maximum eigenvalue is unique and bounded away from the remaining eigenvalues. Nevertheless the size of the second largest eigenvalue is influential in determining such matters as the rate of convergence of the technique of successive squaring, and in any event governs the rate of approach to the equilibrium eigenvector when the matrix is applied iteratively to a trial vector.

There are two familiar formulations for bounds on the modulus of the second eigenvalue (which neither has to be real nor unique). One is essentially equivalent to using the spectral theorem to subtract out the projection operator belonging to the largest eigenvalue in order to apply the Gerschgorin limits anew [20, p. 51]. The second interprets the matrix as an operator on a projective space, for which the largest eigenvector becomes a fixed point and the remaining eigenvalues refer to movement within the projective space.

The second approach is quite reasonable considering that eigenvectors in linear spaces correspond to fixed points in projective spaces. The stability of the fixed point is determined to a certain extent by the Jacobian — corresponding to the derivative — of the mapping at the fixed point, but in more detail by considering the remaining eigenvalues individually. In other words, the Jacobian matrix rather than just the Jacobian determinant should be consulted.

Birkhoff [22] has emphasized the projective point of view, but the most accessible account is probably the painstaking derivation from first principles by Bauer [23].

In any event, suppose that $\mathbf{A}$ is a strictly positive matrix for which

$$K = \max_{ijkl} \sqrt{\frac{a_{ij}a_{kl}}{a_{il}a_{kj}}}$$

$$M = \max_{ij} a_{ij}$$

$$m = \min_{ij} a_{ij}$$

and that $\rho(A)$ is the Frobenius-Perron, or dominant, eigenvalue of $\mathbf{A}$. Then any other eigenvalue $\lambda$ must satisfy

$$|\lambda| \leq \frac{K-1}{K+1}\rho(A) \leq \frac{M-m}{M+m}\rho(A).$$

Hopf [24] obtained an alternative version,

$$|\lambda| \le \frac{K-1}{K+1}\rho(A) \le \frac{M^2-m^2}{M^2+m^2}\rho(A).$$

The bounds for both estimates are actually attained for certain matrices, making them optimal in the absence of further information concerning $\mathbf{A}$. When the eigenvector corresponding to $\rho(A)$ is known, some further improvement is possible [25].

These results would not apply directly to a de Bruijn matrix because of its sparsity. Yet it has a power filled solidly with 1's whose oscillation vanishes, forcing the second largest eigenvalue of the power to be identically zero, in agreement with the characteristic equation. Less extreme conclusions govern probabilistic de Bruijn matrices, but uniformity would still surely speed any approach to equilibrium.

### 12.4 Equilibrium eigenvector

Crude estimates of the equilibrium eigenvector may be obtained by successive squaring, but better estimates are usually needed. A fairly recent article [26] utilizes an approximation to the matrix resolvent — itself both an eigenvector matrix and a positive matrix for a suitable range of its parameter — to characterize polyhedra confining the equilibrium eigenvector. Namely, if $\mathbf{L}$ is a positive matrix of lower bounds to the matrix $\mathbf{A}$, and $\lambda$ is an upper bound to $\rho(A)$, the rows (or columns) of the resolvent

$$R(\lambda) = (\lambda I - L)^{-1}$$

can be used to form the cages.

## 13 Determinant and inverse

A doubly stochastic one-stage de Bruijn diagram would have a probability matrix

$$\mathcal{P}_1 = \begin{bmatrix} p & q \\ q & p \end{bmatrix}$$

with $q = 1 - p$, whose eigenvalues would be $\lambda = 1, p - q$; being symmetric, the matrix of both left and right eigenvectors would be

$$\frac{1}{2}\begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}.$$

The probability matrix of a two stage diagram is a little more complicated.

$$\mathcal{P}_2 = \begin{bmatrix} p_1 & q_2 & \cdot & \cdot \\ \cdot & \cdot & p_3 & q_4 \\ q_1 & p_2 & \cdot & \cdot \\ \cdot & \cdot & q_3 & p_4 \end{bmatrix}$$

with $q_i = 1 - p_i$, and the characteristic polynomial

$$\lambda^4 - \lambda^3(p_1 + p_4) - \lambda^2(p_1 p_4 - p_2 p_3) +$$

$$\lambda(p_2 d_{34} + p_3 d_{12}) - d_{12} d_{34}.$$

with two determinants defined by

$$\begin{aligned} d_{12} &= (p_1 p_2 - q_1 q_2) \\ d_{34} &= (p_3 p_4 - q_3 q_4) \end{aligned}$$

The determinant of the de Bruijn matrix is the product of two smaller determinants corresponding to the evident blocks in the de Bruijn matrix; in this we have a special case of a quite general result. The $p$'s and $q$'s were defined as they are with the thought of equating the subscript pairs (1,2) and (3,4) to get a doubly stochastic matrix, but the best interpretation of the vanishing of the small determinants is that the biases of the probabilities in their submatrices are equal.

The constant term in the characteristic equation will be zero, giving a single zero root, if either determinant is zero. The coefficient of $\lambda$ will also be zero if both are zero, producing a double zero root. In order to get three equal roots and thus open up the possibility of the Jordan normal form, requires some similarity between the two submatrices in addition.

The representations of the de Bruijn matrix as sums and products need very little change to apply to the probabilistic versions as well. The factorizations give immediate formulas for determinants; when they do not vanish, the block diagonal form of of one of the factors, together with the fact that the other is a permutation matrix quickly reveals a form for the inverse matrix. Taking as an example the matrix of the last section, we have

$$\mathcal{P}_2^{-1} = \begin{bmatrix} \frac{p_2}{d_{12}} & \cdot & \frac{-q_2}{d_{12}} & \cdot \\ \frac{-q_1}{d_{12}} & \cdot & \frac{p_1}{d_{12}} & \cdot \\ \cdot & \frac{p_4}{d_{34}} & \cdot & \frac{-q_4}{d_{34}} \\ \cdot & \frac{-q_3}{d_{34}} & \cdot & \frac{p_3}{d_{34}} \end{bmatrix}.$$

The Gerschgorin limit of this matrix requires its maximum eigenvalue to be less than the greatest reciprocal determinant $1/d_{12}$ or $1/d_{34}$ (all with respect to absolute values). Generalizing, this means that *every* eigenvalue of $\mathcal{P}_n$ must be

greater than the lesser of these determinants. Of course, if one of them is zero, we know that the lower bound is reached and $\mathcal{P}_n$ is singular.

In the other direction, unless some $p_i$ or $q_i$ is zero, every matrix element of $\mathcal{P}_n^n$ will be strictly positive, although in the probabilistic case no two of them have to be equal. This ensures that the maximum eigenvalue, $\lambda = 1$, will be unique. Conversely, if some probability or coprobability vanishes, the possibility of degeneracy exists (but is not obligatory).

# 14 Chacteristic equation

Unfortunately information about the other eigenvalues, particularly the second largest of them, is not so readily available—either directly or from the factored forms. However, formulas for the coefficients of the characteristic equation can be derived from the symbolic form of the de Bruijn matrix elements; their expression is even more elegant if a new rule of composition is introduced for regular expressions, particularly for sequences of symbols.

## 14.1 Merged product

Let us suppose $a$ and $b$ are letters, and that $x$ is a sequence, possibly null and possibly empty. We define the merged product of the sequences $s$ and $t$, denoted $s \vee t$, by

$$s \vee t = \begin{cases} axb & s = ax \text{ and } t = xb \\ \phi & \text{otherwise} \end{cases}$$

Likewise, define the overlap, $s \wedge t$, by

$$s \wedge t = \begin{cases} x & s = ax \text{ and } t = xb \\ \phi & \text{otherwise} \end{cases}$$

These are just the combinations of indices required to work with the de Bruijn matrices. For example, the $2^n \times 2^n$ column-stochastic matrix is defined in terms of $n$- and $(n+1)$-block probabilities by the formula

$$[\mathcal{C}_n]_{ax,yb} = \begin{cases} \frac{p(ax \vee yb)}{p(ax)} & p(ax) \neq 0 \\ 0 & \text{otherwise} \end{cases}$$

Correspondingly the row-stochastic matrix is defined by

$$[\mathcal{R}_n]_{ax,yb} = \begin{cases} \frac{p(ax \vee yb)}{p(xb)} & p(xb) \neq 0 \\ 0 & \text{otherwise} \end{cases}$$

Unless stated otherwise, we will assume that a probabilistic de Bruijn matrix is column-stochastic. Since it is not always convenient to show the matrix

elements as a quotient, but it is essential to know which of them intrinsically vanish, let us write

$$[\mathcal{C}_n]_{ax,yb} = m(ax, yb)$$

and note that it vanishes unless $x = y$, or alternatively when $ax \vee yb = \phi$.

## 14.2 Trace

The trace of $\mathcal{C}_n$, which is the coefficient of $\lambda^{n-1}$ in the characteristic equation, satisfies

$$\begin{aligned} Tr(\mathcal{C}) &= \sum_{ax} m(ax, ax) \\ &= \sum_{i\,|ax=xi} m(ax, xi) \\ &= \sum_{i} m(i^*, i^*) \end{aligned}$$

The essential element in all of these calculations is to factor the column index in such a way that it can match a row index and yet produce a non-zero merged product.

## 14.3 second coefficient

$$\begin{aligned} a_2 &= \sum_{ax \le by} (m(ax, ax)m(by, by) - \\ &\quad m(ax, by)m(by, ax)) \\ &= \sum_{i\,|ax=xi} \sum_{j\,|by=yj} m(ax, xi)m(by, yj) - \\ &\quad \sum_{i\,|by=xi} \sum_{j\,|ax=yj} m(ax, xi)m(by, yj) \\ &= \sum_{i \le j} m(i^*, i^*)m(j^*, j^*) - \\ &\quad \sum_{i \le j} m((ij)^*)m((ji)^*) \\ &= \sum_{i \le j} \begin{vmatrix} m(i^*, i^*) & m((ij)^*) \\ m((ij)^*) & m(j^*, j^*) \end{vmatrix} \end{aligned}$$

In essence, this sum runs over all cycles of length 2 in the de Bruijn diagram. The solution to the requirements $by = xi$ and $ax = yj$ is $y = (ab)^*$; however this notation must be understood to designate only as much of the sequence as is needed. Thus $(01)^*$ could represent 0, 01, 010, 0101, and so on, but not 101, for example.

### 14.4 principal minors

Striking out rows and columns intersecting on a diagonal will always leave some surviving elementary determinants, until so many have been stricken out that it is no longer possible to form a complete determinant. The coefficient of the elementary determinants will depend on how much of the remaining elementary determinant can be salvaged.

In general, the determinant of the de Bruijn $|m(ix, yj)|$ factorizes, so that

$$|m(ix, yj)| = \prod_{x,x} |m(ix, xj)|,$$

where the factors are $k \times k$ determinants obtained by varying the indices $i$ and $j$ with fixed $x$. To get the minor of the $hz, hz$ diagonal element, we need to consider two cases. If this pivot does not belong to any subdeterminant, it can be ignored. If it does, we drop the $z, z$ term from the product, replacing it by the internal minor from within the omitted factor. Thus

$$a_1 = \sum_{hz=wh} cofactor(m(hz, hz)) \prod_{x \neq z} |m(ix, xj)|.$$

### 14.5 determinant

Although we already have the determinant of the probabilistic de Bruijn matrices from their factored forms, it is worth observing that it can be calculated directly by following the symbolic procedure.

$$|m(ix, yj)| = \prod_{x,x} |m(ix, xj)|,$$

## 15 Summary

In conclusion, there are two aspects of graph theory which are important for automata theory. One, typified by the use of classical de Bruijn diagrams and their subdiagrams, portrays the relationships between components of the automaton, such as the individual neighborhoods or partial neighborhoods, and the evolution of the automaton. This application emphasizes several aspects of graph theory, motivating the introduction of operations on graphs which adequately describe properties of the automaton.

Among these are the ordering of graphs, homomorphisms between graphs, and such operations as the formation of cartesian products and dual graphs. The characterization of homomorphism in terms of matrices embodied in Equations 3 and 16 has long been known to mathematicians with varying degrees of formality, but deserves to be emphasized anew. The definition of duals via the $RC$ factorization is more original, probably because it relates better to "digraphs" than to the structure traditionally called a graph.

Consequently, it is a step away from the classical treatments of graph theory, such as Ore's *American Mathematical Society* monograph [27]; treatments which were more content with simply describing and classifying graphs.

Not only that, but the requirements of the application to automata theory oblige us to consider several alternative approaches to graphs not ordinarily considered part of graph theory, such as the description of graphs by symbolic equations, and their representation by regular expressions. Likewise the topological matrix, or connectivity matrix, is intimately related to properties considered essential to the understanding of automata, requiring a working knowledge of the class of positive matrices.

The second aspect of graph theory concerns its relation to probability theory, via the topological matrix, probabilistic evolution, and probabilistic de Bruijn diagrams. Strictly, interest lies in the application of detailed properties of positive matrices and the Frobenius-Perron theory to all the structures which have been constructed with the aid of graph theory in the earlier sections of the article.

Probabilistic de Bruijn matrices describe correlations between overlapping cell blocks in an automaton. Yet another class of diagram, evolution diagrams, has its probabilistic version; thus either type of diagram has a probabilistic version which could be of concern. Some interesting recently published papers have dealt with establishing and then solving equations for self-consistent probabilities for clusters of cells [28, 29].

So, although it is not part of graph theory, automata theory brings about an interesting application of the classical Perron-Frobenius theory to certain classes of graphs — the de Bruijn diagrams and evolutionary diagrams — which might otherwise have escaped such attention; and in the process some interesting new characteristics of graphs are revealed.

## acknowledge

This article is an expanded version of an invited address presented to the "$4^o$ Coloquio de teoría de las gráficas, combinatoria, y sus aplicaciones," Puebla, February 20-24 1989.

## References

[1] Claude E. Shannon, "Mathematical Theory of Communication," *Bell System Technical Journal* **27** 379-423, 623-658 (1948).

[2] W. S. McCulloch and W. Pitts, "A logical calculus of the ideas immanent in nervous activity," *Bulletin of Mathematical Biophysics* **5** 115-133 (1943).

[3] John H. Conway, *Regular algebra and finite machines*, Chapman and Hall, London, 1971.

[4] R. C. Backhouse and B. A. Carré, "Regular Algebra Applied to Path-finding Problems," *Journal of the Institute for Mathematics and its Applications* **15** 161-186 (1975).

[5] Robert L. Hemminger and Lowell W. Beineke, "Line graphs and line digraphs," *in* Lowell W. Beineke and Robin J. Wilson, *Selected Topics in Graph Theory*, Academic Press, New York, 1978. (ISBN 0-12-086250-6) pp. 271-305

[6] Paul I. Richards, "Precedence constraints and arrow diagrams," *SIAM Review* **9** 548-553 (1967).

[7] Solomon W. Golomb, *Shift Register Sequences*, Holden-Day, Inc., San Francisco, 1967.

[8] Anthony Ralston, "De Bruijn Sequences—A Model Example of the Interaction of Discrete Mathematics and Computer Science," *Mathematics Magazine* **55** 131-143 (1982).

[9] Stephen Wolfram, "Statistical mechanics of cellular automata," *Reviews of Modern Physics* **55** 601-644 (1984).

[10] Stephen Wolfram, "Computation theory of cellular automata," *Communications in Mathematical Physics* **96** 15-57 (1984).

[11] Wentian Li, "Power spectra of regular languages and cellular automata," *Complex Systems* **1** 107-130 (1987).

[12] Masakazu Nasu, "Local Maps Inducing Surjective Global Maps of One-Dimensional Tessellation Automata," *Mathematical Systems Theory* **11** 327-351 (1978).

[13] Erica Jen, "Cylindrical Cellular Automata," *Communications in Mathematical Physics* **118** 569-590 (1988).

[14] I. J. Good, "Normal recurring decimals," *Journal of the London Mathematical Society* **21** 169-172 (1946).

[15] N. G. de Bruijn, "A combinatorial problem," *Koninklijke Nederlands Akademie van Wetenschappen, Proceedings* **49** 758-764 (1946).

[16] Marshall Hall, Jr., *Combinatorial Theory*, Blaisdell Publishing Company, Waltham, Massachusetts, 1967.

[17] Edward F. Moore, "Gedanken Experiments on Sequential Machines," in *Automata Studies,* C. E. Shannon and J. McCarthy, eds., Princeton University Press, Princeton, 1956.

[18] Richard S. Varga, *Matrix Iterative Analysis*, Prentice Hall, Inc, Englewood Cliffs, New Jersey, 1962.

[19] Eugene Seneta, *Non-Negative Matrices*, John Wiley and Sons, New York, 1973. (ISBN 0-470-77605-6)

[20] Abraham Berman and Robert J. Plemmons, *Nonnegative Matrices in the Mathematical Sciences*, Academic Press, New York, 1979. (ISBN 0-12-092250-9)

[21] Henryk Minc, *Nonnegative Matrices*, John Wiley and Sons, New York, 1988. (ISBN 0-471-83966-3)

[22] Garrett Birkhoff, "Extensions of Jentzsch's Theorem," *Transactions of the American Mathematical Society* **85** 219-227 (1957).

[23] F. L. Bauer, "An Elementary Proof of the Hopf Inequality for Positive Operators," *Numerische Mathematik* **7** 331-337 (1965).

[24] Eberhard Hopf, "An Inequality for Positive Linear Integral Operators," *Journal for Mathematics and Mechanics* **12** 683-692 (1963).

[25] F. L. Bauer, E. Deutsch, and J. Stoer, "Abschätzungen für die Eigenwerte positiver linearer Operatoren," *Linear Algebra and its Applications* **2** 275-301 (1969).

[26] P-. J. Courtois and P. Semal, "Bounds for the Positive Eigenvectors of Nonnegative Matrices and for their Approximations by Decomposition," *Journal of the Association for Computing Machinery* **31** 804-825 (1984).

[27] Oystein Ore, *Theory of Graphs,* American Mathematical Society, Providence, Rhode Island, 1962. (ISBN 0-0218-1038-3)

[28] Howard A. Gutowitz, Jonathan D. Victor, and Bruce W. Knight, "Local structure theory for cellular automata," *Physica* **28D** 18-48 (1987).

[29] W. John Wilbur, David J. Lipman, and Shihab A. Shamma, "On the prediction of local patterns in cellular automata," *Physica* **19D** 397-410 (1986).