Non-equilibrium Digits Model

Considering a string of digits/letters etc. with each such string (potentially up to some symmetries) being considered a microstate of the system. In the simplest case it seems logical to focus on models where changing any one digit is one transition.

1 Binary Strings with Single Digits Transitions dependent on NNs

The simplest place to start seems to be binary strings with any transition rates only dependent on (up to) its two neighbours (can be chiral). Besides, this we ought to consider what biophysical mechanisms facilitate these transitions. Firstly, these must be affected by the outside environment and these transitions also must affect the outside environment as otherwise by detailed balance any inverse transitions would have to be at the same rate. This means that in a binary model, even if we had different mechanisms for each combination of neighbours, as for each of those the $0 \to 1$ and $1 \to 0$ reactions have the same rate we just get a random string. This means that for each mechanism we will have

$$\text{env} + \overline{?0?} \underset{r_{\text{mech},b}}{\overset{r_{\text{mech},f}}{\rightleftharpoons}} \overline{?1?} + \text{env}' \quad \text{with} \quad \frac{r_f}{r_b} = \exp\{\beta\mu_{\text{mech}}\} \tag{1}$$

with it potentially coupling to different neighbor combinations at different rates which may be given in a matrix K_{mech} such that the reaction rates for

$$\text{env} + \overline{\text{i0j}} \underset{r_{\text{mech},ij,b}}{\overset{r_{\text{mech},ij,f}}{\rightleftharpoons}} \overline{\text{i1j}} + \text{env}' \tag{2}$$

are given by

$$r_{\text{mech},ij,f} = K_{\text{mech},ij} \frac{\exp(\beta\mu_{\text{mech}})}{\exp(\beta\mu_{\text{mech}}) + 1} \tag{3}$$

$$r_{\text{mech},ij,b} = K_{\text{mech},ij} \frac{1}{\exp(\beta\mu_{\text{mech}}) + 1} \tag{4}$$

in the future different shorthand notations may be used. Also note that in this binary model any forward rate always corresponds to a $0 \to 1$ reaction and vice-versa.

So in summary each mechanism has its μ (originating either from energetics or effects on the outside environment) which sets the balance of 0 to 1 and 1 to 0 rates. And a K which sets the overall rates depending on neighbours of the affected digit. The total rate of a particular transition is then a sum over all the mechanisms rates which are given by eqs. (3) and (4). Also, worth noting is the case of a mechanism being maximally driven, this results in that given mechanism only facilitating 0 to 1 or 1 to 0 transitions and is perhaps the most intuitive unit to start looking at.

1.1 Symmetries and K

Firstly, to reduce the number of different setups we have to consider examine the symmetries which in particular affect K. The only one that is always present is exchanging all 0s and 1s. For any K this comes down to a point reflection around the middle of the matrix. Thus, if any two configurations have all Ks such that they are such reflections of each other than those systems will have the same behaviours just with all their respective microstates being related by exchanging all 0s and 1s.

More conceptually complex is left right reflection. The way the setup is currently described it is worth noting that the digit strings are implicitly oriented, meaning we do not consider 10011 and 11001 to be the same string. This is the simplest way of working and does allow for chiral systems, in a biological sense this corresponds to something along the lines of squares and circles being placed on an explicitly oriented arrow. The corresponding transformation of the Ks is to take their transpose, so similarly to before two systems where all Ks are transposes of each other will have the "same" behaviour.

Another, optional symmetry of sorts is worth noting and that is offsets and whether we consider the string to be looped or a chain with boundaries. We mostly look at loop geometries meaning we consider the leftmost digit to be the right neighbour of the rightmost digit and vice-versa. That said, we do not reduce the microstates, as in we do consider 0001 and 0010 to be different microstates, they just will have the same sort of interactions. I do believe this is the correct way of doing things here as it accounts for the entropic factors of the biophysical microstates. I am not quite sure at this point what the best way is to deal with chain geometries, but could involve more parameters.

The left right symmetry is worth addressing in more detail. If we wanted to work on squares and circles on an unoriented line instead then I think one valid way of adjusting the Ks correctly is to do $K_{ij} \to K_{ij} + (1 - \delta_{ij})K_{ji}$ (no einsum) which corresponds to allowing the hypothetical enzyme to flip itself and still work. Alternatively, one can just consider all the hypothetical enzymes to not know about this direction which is just equivalent to choosing only symmetric Ks. Ultimately which of these is appropriate depends on if there are really 2 enzymes one for each direction and the string loses its direction, or is there only one enzyme which just cannot tell read the direction of the string.

1.2 Single mechanism

Notably, this cannot give rise to an out-of-equilibrium system, but it is still worth exploring. This gives us a single μ and K, leaving μ be for a bit, what options do we have for K. If we at first only allow $K_{ij} \in \{0, 1\}$ we have 2^4 options however many show the same behaviour due to the symmetries described above. All the others are enumerated in table 1. Note that all of the arrows here are double-headed, that said that is assuming finite μ. μ essentially biases a mechanism towards turning 0s to 1s or otherwise, if it is 1 0 then it is unbiased but taking limits to $\pm\inf$ can make a mechanism affect only one direction.

1.3 Connection to cellular automata

Since this is model does seem similar to cellular automata it is worth investigating the connection. Classic CE are deterministic and so for each possible transition of a to b with neighbours i and j the transition is either always going to happen or never. This largely corresponds to the $\mu \to \pm\inf$ limits. Note however that for a single mechanism all such transitions would have to point in the same direction and hence we can not achieve all the systems corresponding to all difference CEs using only a single mechanism. However, given that we can tune individually the rates (or in the simpler case enable/disable them) based on each neighbour combination using K, we can achieve all CE corresponding systems in our model using two mechanisms each biased in the opposite direction. For a simple sanity check note that as dicussed before if we only consider entries of 0 or 1 then there are a total of 2^4 possible Ks hence $2^4 \times 2^4$ total different combinations of 2 K matrices. This agrees with the 2^8 different basic CE rules.

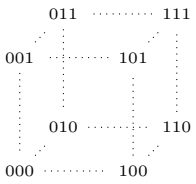
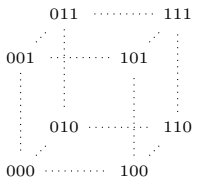
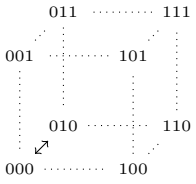
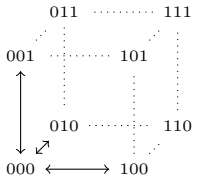
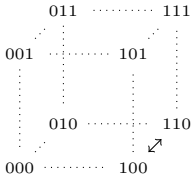
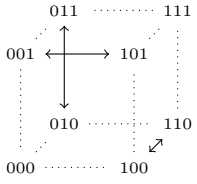
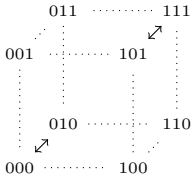
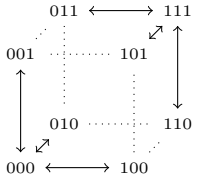
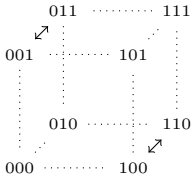
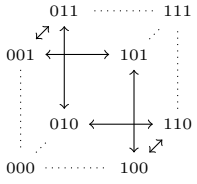
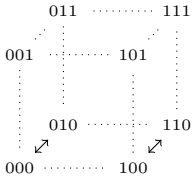
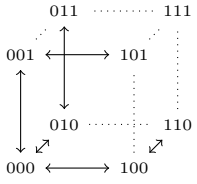
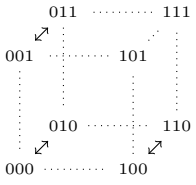
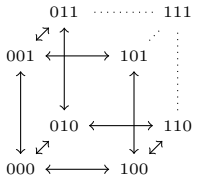
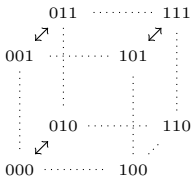
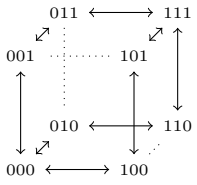
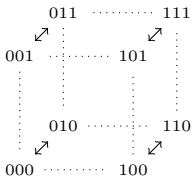
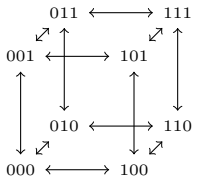
K	transitions	degen., sym.	Elementary trans.	All $N = 3$ trans.
$\begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix}$	none	1, none		
$\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$	$000 \leftrightarrow 010$	2, via $0 \leftrightarrow 1$		
$\begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}$	$100 \leftrightarrow 110$	2, via either		
$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$	$000 \leftrightarrow 010$ $101 \leftrightarrow 111$	1, none		
$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$	$001 \leftrightarrow 011$ $100 \leftrightarrow 110$	1, none		
$\begin{pmatrix} 1 & 0 \\ 1 & 0 \end{pmatrix}$	$000 \leftrightarrow 010$ $100 \leftrightarrow 110$	4, via combinations of both		
$\begin{pmatrix} 1 & 1 \\ 1 & 0 \end{pmatrix}$	all except $101 \leftrightarrow 111$	2, via $0 \leftrightarrow 1$		
$\begin{pmatrix} 1 & 1 \\ 0 & 1 \end{pmatrix}$	all except $100 \leftrightarrow 110$	2, via either		
$\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}$	all	1, none		

Table 1: Summary of all the possible Ks for N=3 and a single mechanism with a unique behaviour.

2 Binary, NN, Cellular Automata like Systems

These are a type of the models discussed above where as discussed before we have two mechanisms, one biased towards 0 to 1 transitions with its matrix $K_{01} = U$ and the other biased towards 1 to 0 transitions with its matrix $K_{10} = D$.

2.1 Symmetries of the CA system

As discussed before we have two main symmetry operations we consider, exchanging all 0s to 1s and vice-versa (01) and reversing the string (LR). Naturally then we can also do both, veiwing this as a symmetry group I label these operations as g, h and $f = gh = hg$ as verified by making a multiplication table. These operations then transform the two matrices U and D as

$$g \leftrightarrow \begin{pmatrix} a & b \\ c & d \end{pmatrix} \begin{pmatrix} e & f \\ g & h \end{pmatrix} \rightarrow \begin{pmatrix} h & g \\ f & e \end{pmatrix} \begin{pmatrix} d & c \\ b & a \end{pmatrix} \tag{5}$$

$$h \leftrightarrow \begin{pmatrix} a & b \\ c & d \end{pmatrix} \begin{pmatrix} e & f \\ g & h \end{pmatrix} \rightarrow \begin{pmatrix} a & c \\ b & d \end{pmatrix} \begin{pmatrix} e & g \\ f & h \end{pmatrix} \tag{6}$$

$$f \leftrightarrow \begin{pmatrix} a & b \\ c & d \end{pmatrix} \begin{pmatrix} e & g \\ f & h \end{pmatrix} \rightarrow \begin{pmatrix} h & f \\ g & e \end{pmatrix} \begin{pmatrix} d & b \\ c & a \end{pmatrix} \tag{7}$$

The symmetry group as Abelian with $g^2 = h^2 = f^2 = e$ and combining any of the two gives the third.

These symmetries are useful for two things, firstly narrowing down many different CA rules to only those which show distinctive behaviour. In practice this means that if two rules are related by a symmetry operation then only one is worth investigating. Numerically, I have checked there are 88 rule classes based on these symmetries, each having between 1 and 4 different rules. Secondly, we can then look for those rules that are invariant under some or all of these operations.

2.2 Symmetry and equilibrium classes

Any particular CA like rule can be classified according to the discussed symmetries in one of 5 classes. Either a rule is not symmetric under any of the operations, or it is symmetric under precisely one of g, h and f, or it is symmetric under all of them. In addition to this it is also worth classifying according to whether a rule is an equilibrium one or not, this is the case iff $U = D$. See table 2.

Symmetries	General form of Ks plus conditions	d.o.f.	#rules	Ks at eq. plus conditions
All	$\begin{pmatrix} a & b \\ b & c \end{pmatrix} \begin{pmatrix} c & b \\ b & a \end{pmatrix}$ always	3	8/8	$\begin{pmatrix} a & b \\ b & a \end{pmatrix}$ always
h only	$\begin{pmatrix} a & b \\ b & c \end{pmatrix} \begin{pmatrix} e & f \\ f & g \end{pmatrix}$ iff $(a \neq e) \vee (b \neq f) \vee (c \neq g)$	6	56/28	$\begin{pmatrix} a & b \\ b & c \end{pmatrix}$ iff $a \neq c$
g only	$\begin{pmatrix} a & b \\ c & d \end{pmatrix} \begin{pmatrix} d & c \\ b & a \end{pmatrix}$ iff $b \neq c$	4	8/4	$\begin{pmatrix} a & b \\ b & a \end{pmatrix}$ so never
f only	$\begin{pmatrix} a & b \\ c & d \end{pmatrix} \begin{pmatrix} d & b \\ c & a \end{pmatrix}$ iff $\neq c$	4	8/4	$\begin{pmatrix} a & b \\ c & a \end{pmatrix}$ ff $a \neq c$
None	$\begin{pmatrix} a & b \\ c & d \end{pmatrix} \begin{pmatrix} e & f \\ g & h \end{pmatrix} \ldots$	8	176/44	$\begin{pmatrix} a & b \\ c & d \end{pmatrix} \ldots$

Table 2: Symmetry classes of the CA type systems along with some of their properties. All columns except the last do not distinguish between in and out of equilibrium. The rules column is the number of rules in the class before accounting for other symmetries and after.

2.2.1 Fully symmetric rules

From table 2 we can start looking at the particular rules in some of the classes, the most symmetric begin the natural first choice. Note that all of these are fully symmetric and so have no other rules that are similar to them, hence all are worth looking at. These rules are summarized in

Code	Ks	# trans.	is at eq.	is interesting/notes
77	$\begin{pmatrix}1&0\\0&0\end{pmatrix}\begin{pmatrix}0&0\\0&1\end{pmatrix}$	2	no	
232	$\begin{pmatrix}0&0\\0&1\end{pmatrix}\begin{pmatrix}1&0\\0&0\end{pmatrix}$	2	no	
150	$\begin{pmatrix}0&1\\1&0\end{pmatrix}\begin{pmatrix}0&1\\1&0\end{pmatrix}$	4	yes	
105	$\begin{pmatrix}1&0\\0&1\end{pmatrix}\begin{pmatrix}1&0\\0&1\end{pmatrix}$	4	yes	
178	$\begin{pmatrix}0&1\\1&1\end{pmatrix}\begin{pmatrix}1&1\\1&0\end{pmatrix}$	6	no	
23	$\begin{pmatrix}1&1\\1&0\end{pmatrix}\begin{pmatrix}0&1\\1&1\end{pmatrix}$	6	no	
204	$\begin{pmatrix}0&0\\0&0\end{pmatrix}\begin{pmatrix}0&0\\0&0\end{pmatrix}$	0	yes	trivial
51	$\begin{pmatrix}1&1\\1&1\end{pmatrix}\begin{pmatrix}1&1\\1&1\end{pmatrix}$	8	yes	trivial

Table 3: Summary of all of the fully symmetric CA rule systems. #tran. refers to the number of elementary transitions.