

## 1 PN - qualitative invariants

We study Petri nets equilibrium with an eye on developing this later for the more sophisticated modeling languages Kappa. We will keep the same notations when possible.

### 1.1 PN - Basic definition

A Petri net is:

- two finite sets  $P$  (places, species),  $T$  (transitions, reactions),
- an input (consumption) and output (production) function  $(i, o) : P \times T \rightarrow \mathbb{N} \times \mathbb{N}$

The idea is that places hold a certain number of agents of a certain species, and  $i(p, t)$  is the number agents of species  $p$  that reaction  $t$  consumes, while  $o(p, t)$  is the number it produces.

There is a redundant terminology which witnesses the history of the subject. I will mostly use the chemical side of the dictionary

The state space is  $P \rightarrow \mathbb{N} \simeq \mathbb{N}^P$  (aka markings, multisets over

$P$ , integer vectors of size  $|P|$ ). As functions, states can be added, subtracted and compared (they have a linear ordered structure).

## 1.2 Computations

A computation step labelled by  $r \in T$  (aka a firing of  $r$ ) is:

$$s \longrightarrow_r s + o(r) - i(r) \text{ if } s \geq i(r)$$

where  $\geq$  is the pointwise order on finite functions, and the precondition  $s \geq i(r)$  expresses the fact that the reaction needs a minimal amount of inputs to fire.

This defines a transition system (TS) on the state space, that is to say a binary relation on  $\mathbb{N}^P$  labelled in  $T$ .

This TS is *monotonic* in the sense that  $s \rightarrow_r s' \Rightarrow s + t \rightarrow_r s' + t$  for any  $t \in \mathbb{N}^P$  (more tokens never inhibit a transition - a key ingredient in the simplicity of the TS, inhibitory reactions make the entire framework a lot more complex and powerful).

### 1.3 Matrix representation

Write  $p = |P|$ ,  $q = |T|$ .

If  $M : a \leftarrow b$  is a matrix, then  $M^t : b \leftarrow a$  is its transpose.

States form a subset of the real vector space  $\mathbb{R}^P$  of dimension  $p$ ; they are closed under linear combination with integer coefficients.

We can represent the input and output functions as matrices of dimensions  $p \times q$  with coefficients in  $\mathbb{N}$ , and define the (stoichiometric) matrix  $C : p \leftarrow q$  as  $o - i$ ; that is to say  $c_{ij} \in \mathbb{N} =$  production of species of type  $i$  by reaction/transition  $j$ .

We write  $r_j$  for the canonical basis of  $\mathbb{R}^q$ , and  $r_j \cdot y$  for the effect of reaction  $j$  on  $y \in \mathbb{N}^p$ .

By definition of  $C$ ,  $r_j \cdot y - y = Cr_j$  (when  $r_j$  is applicable to  $y \in \mathbb{N}^p$ , ie when  $i(r_j) \leq y$ ) - that is to say  $Cr_j$  is the net effect of applying  $r_j$  which is independent of the state one applies it to (and of the manner in which one applies it - more later); what depends on the state is the application condition  $s \geq i(r_j)$ .

A vector  $x \in \mathbb{N}^q$  represents a linear combination of reactions and

$Cx$  is just the total resulting production as  $Cr_j(i) = c_{ij}$  is indeed the production of  $i$  by reaction  $j$ .

#### 1.4 examples

In practice we present a Petri net as a list of reactions, here are 3 examples:



#### 1.5 transition invariants

A *transition invariant* is an  $x \in \mathbb{N}^q$  such that  $Cx = 0$ . Equivalently a combination of rules  $x$  such that, wherever applicable, the underlying state  $s$  is unchanged.

Eg in the example (3), we have an invariant  $x^t = (1 \ 1)$ . It corresponds to loops starting from any state where  $I > 0$ .

In general, a combination of rules  $x$  corresponds to countably many trajectories in the underlying state space  $\mathbb{N}^P$ ; specifically, any trajectory such that one has enough tokens all along some sequencing/scheduling  $\tilde{x}$  of  $x$ , meaning  $\tilde{x}$  is a sequence of reactions that projects to the multiset  $x$  by forgetting its ordering; cf PN monotony.

### 1.6 place invariants

A vector  $y \in \mathbb{N}^p$  can be seen as a marking (aka a state), but what is  $C^t y$  then?

A *place invariant*, is an  $u \in \mathbb{R}^p$  such that for all reactions  $j$ , and all states  $y$  (where  $j$  applies):

$$u^t(r_j \cdot y) - u^t y = u^t C r_j = 0$$

which is equivalent to

$$C^t u = 0 : 1 \rightarrow q$$

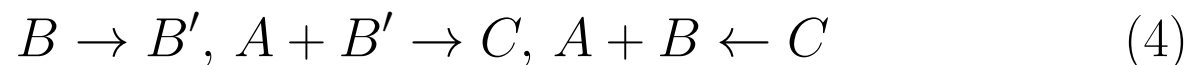
As all solutions to the above will have rational coefficients, we can always choose  $u \in \mathbb{N}^p$  by multiplying by a well-chosen ppcm.

Suppose  $A \rightarrow 2B$  is the only reaction, then  $C^t = (-1 \ 2)$ , so  $C^t u = 0$  ie  $u^t \propto (2 \ 1)$  and indeed  $u^t y = 2y_A + y_B$  is (a place) invariant.

We can think of  $u$  as a pricing such that any transformation/reaction is neutral (if it is an invariant); in general  $u^t C y = (C^t u)^t y$  measures the global price of doing  $y$  measured with  $u$ .

### 1.7 A more exciting example

Consider:



we can compute and interpret the P-invariants from:

$$(u_A u_B u_{B'} u_C) \begin{pmatrix} 0 & -1 & 1 \\ -1 & 0 & 1 \\ 1 & -1 & 0 \\ 0 & 1 & -1 \end{pmatrix} = 0$$

which gives a solution space of dimension 2,  $u_B = u_{B'}$ ,  $u_C = u_A + u_B$ , with basis  $u_1^t = (0111)$ ,  $u_2^t = (1001)$  giving respective invariants:

$$\begin{array}{ll} y_B + y_{B'} + y_C & \textit{preservation of } B \\ y_A + y_C & \textit{preservation of } A \end{array}$$

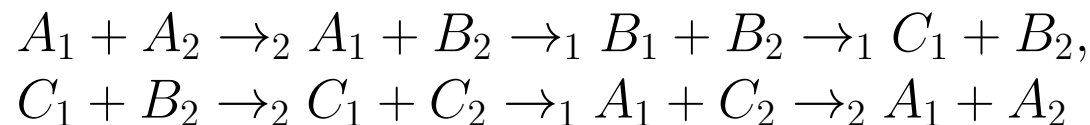
### 1.8 for experts

Consider the following two ‘cooperating’ (ordered)  $T$ -invariants:

$$\begin{array}{l} \phi_1 = A_1 \rightarrow B_1, \mathbf{B}_2 + B_1 \rightarrow \mathbf{B}_2 + C_1, C_1 \rightarrow A_1 \\ \phi_2 = A_2 \rightarrow B_2, \mathbf{C}_1 + B_2 \rightarrow \mathbf{C}_1 + C_2, C_2 \rightarrow A_2 \end{array}$$

$\phi_1$  needs an  $A_1$  and a  $B_2$ ,  $\phi_2$  needs an  $A_2$  and a  $C_1$ .

If we start from  $z_0 = A_1 + A_2$ , none of the loops can complete alone; nevertheless, one can realize  $\phi_1 + \phi_2$ , because  $\phi_1$ ,  $\phi_2$  can exchange intermediates  $\mathbf{B}_2$ , and  $\mathbf{C}_1$ :



## 1.9 simple, reversible

Define:

- *simplicity*: no two transitions have identical jumps (columns in  $C$ ).
- *reversibility*: for every transition  $r$ , there is an inverse transition  $r^*$  with  $i(r^*) = o(r)$  and  $i(r) = o(r^*)$

NB: The notion of reversibility is intensional, ie not a property of the underlying TS. Secondly, if the PN is simple, then there is at most one  $r^*$  per  $r$ , so there is no ambiguity. We can reversibilise a PN by adding  $r^*$ s where we lack one (perhaps with a very small rate). We cannot ‘simplicize’ naturally a PN however, we could select among identical columns but that would be arbitrary.

*§simplicity - caveat*

Simplicity seems an innocuous assumption as one would think that it is enough to add reactions with the same balance, but consider  $\emptyset \leftrightarrow A$  vs.  $A \leftrightarrow 2A$ , they add up only in the case  $m(A) > 0$  -



the overlap is not uniform on the state space - so a delicate thing is happening here.

*§Anticipating - somewhat*

simple reversible PNs have infinite time ODE solutions; non simple ones, not so simple! Eg  $2A \rightarrow 3A$  gives  $d/dt A = A^2$ , Ricati's equation with explosive solution  $A(t) = 1/(A(0) - kt)$ ; so reversibility is crucial - indeed  $x' = x^2 - x^3$  is always defined.

*§Two meanings of reversible - caveat*

Let us insist on the difference between the extensional TS and its slightly intensional description via a PN - eg there are two meanings to saying that a PN is reversible: either we mean that the underlying TS or transition graph (TG) is symmetric, or we mean (as we did above) that for every rule there is an inverse rule.

It is not true that if  $N$ 's transition graph is symmetric, then every reaction has an inverse reaction.

Consider:



the TG is (simple but) not symmetric, as we can invert  $r_1$  but not  $r_2$  (at  $1S$ ); but if we add



the TG becomes symmetric (but no longer simple), yet  $r_1$  has no inverse.

What is true is:

**Proposition 1.** *if  $N$ 's TG is symmetric and  $N$  is simple, then  $N$  is reversible (every reaction has an inverse reaction)*

Pick some reaction  $r = m_1 \rightarrow m_2$  and apply  $r$  at state  $m_1$ , by symmetry there must be another reaction  $r' = m'_2 \rightarrow m'_1$  such that:

$$\begin{aligned} m'_2 &\leq m_2 \\ m_2 - m'_2 &= m_1 - m'_1 \end{aligned}$$

if we set  $d := m_2 - m'_2 = m_1 - m'_1$  we have  $r = d + r'^*$  meaning  $r = d + m'_1 \rightarrow d + m'_2$

We can apply the same procedure to  $r'$  obtaining a decomposition  $r' = d' + r''^*$  therefore  $r = d + d' + r''$ , and since  $N$  is simple,  $d = d' = 0$ , which implies that  $r'$  is inverse to  $r$ .  $\square$

Note that the counterexample above corresponds to the proof with  $r = r_1$ ,  $r' = r_2$  and  $r'' = r_3$ ,  $d = I$ ,  $d' = \emptyset$ .

## 2 PN - stochastic semantics

We want to equip our Petri nets with a probabilistic semantics, ie associate to them a ctMC with the same state space and underlying transition graph. PNs have a countably infinite state space and finitely many jumps - so they fit the notion of ctMC equilibrium we have defined previously, and we can study their equilibrium (next section).

In fact, we can define two very different stochastic semantics on

the same PN.

Given a set of *reaction rate constants* - that is to say a map  $k : T \rightarrow \mathbb{R}^+$  - we can define two notions of jumping rate:

- $s \xrightarrow{r} s + o(r) - i(r)$  with rate  $\tau(s, r) = k(r)$
- $s \xrightarrow{r} s + o(r) - i(r)$  with rate  $\tau(s, r) = k(r) \times [i(r); s]$

where  $[i(r); s]$  is the number of ways in which one can select the inputs  $i(r)$  in  $s$ , that is to say:

$$[i(r); s] = \prod_{A \in P} [i(r)(A); s(A)] = \prod_{A \in P} \frac{s(A)!}{(s(A) - i(r)(A))!} \quad (5)$$

We have chosen  $[a; b] = b!/(b-a)!$  the number of injections of  $a$  in  $b$ . Sometimes, one takes as a counting principle  $\{a; b\} = \binom{b}{a}$  instead, ie the number of subsets, but that is inherently a bad convention as we will see when we consider the rule-based extension of PNs.

Anyway,  $\{a, b\} = [a; b]/a!$  so the difference between the two conventions is independent of the state (ie it is static), and can (therefore) be entirely hidden in the rate constant  $k(r)$ .

The second semantics is called *mass action*, this is the one that

interests us.

Note that this defines a compound jump rate:

$$\tau(s, s') = \sum_{\{r|r \cdot s = s'\}} \tau(s, r)$$

If the PN is not simple, distinct reactions may lead to the same result (it is enough that they both apply and have the same balance  $Cr_i = Cr_j$ ; if they are strictly equal -as reactions - we can aggregate them). As we will see this would create a problem when it comes to constructing equilibria (which is why we restrict to simple PNs).

### 3 Petri Net equilibrium

Let  $N$  be a Petri net with species  $S$ , reactions  $R$ , and stoichiometric matrix  $C$ .

We assume  $N$  is *simple* (no two column vectors of  $C$  are identical) and *symmetric* (every column vector  $r$  has a designated opposite vector  $r^*$  - unique by simplicity), and is equipped with *mass action semantics*.

In short  $N$  is *sisma*.

We write  $K$  for  $N$ 's *transitional energy* vector  $K(r) := \log k(r^*)/k(r)$ .  
(log stand for the natural logarithm, ie  $\log e = 1$ .)

**Theorem 1.** *A sisma net  $N$  has a global (nowhere zero) equilibrium iff  $K \in \ker(C)^\perp$ .*

Suppose  $p$  is an equilibrium for  $N$ , then one has  $p(x)/p(y) = q(y, x)/q(x, y)$  for any  $x, y$  in the support of  $p$ ,  $|p|$ , and that of  $q$ . We can exploit this to obtain  $p(z)/p(z_0)$  as the product of rates  $q(y, x)/q(x, y)$  along any path from  $z_0$  to  $z$ .

We also have, by definition of mass action:

$$\frac{q(y, x)}{q(x, y)} = e^{K(r)} \cdot \prod_{A \in S} \frac{y(A)!}{x(A)!}$$

where  $r$  is the (unique by simplicity) transition that takes  $x$  to  $y$ .

Put together, for  $\phi$  an  $R$ -labeled path from  $z_0$  to  $z$  within  $|p|$ , and  $\tilde{\phi}$  the associated reaction vector, this gives us:

$$p(z)/p(z_0) = z_0!/z! \cdot e^{-\langle K, \tilde{\phi} \rangle} \tag{6}$$

Note that this form is symmetric, as  $\phi^*$  goes from  $z$  to  $z_0$ , and  $\langle K, \tilde{\phi}^* \rangle = -\langle K, \tilde{\phi} \rangle$ .

So if  $p$  is an equilibrium which is non-zero at  $z_0$  (equivalently at  $z_0$ 's component) then it is unique on this component, and the rhs (equivalently  $\langle K, \tilde{\phi} \rangle$ ) does not depend on the choice of  $\phi$ .

Now suppose  $\phi$  is a loop, then  $\langle K, \tilde{\phi} \rangle = 0$ , meaning:

$$K \perp \{\gamma \in \mathbb{N}^R \mid \exists \phi \in [z_0; z_0] : \phi \models \gamma \wedge z_0 \in |p|\}$$

Since we assume  $p$  is defined everywhere, this means that  $K$  is orthogonal to every reaction vector that is realized by a loop somewhere in the state space, which, by PN monotonicity, means any reaction invariant. (What if  $|p|$  is not the whole state space, can we still say something?)

In other words,  $K \in \ker(C)^\perp$ .

Conversely, if  $K \in \ker(C)^\perp$ , then obviously  $\langle K, \tilde{\phi} \rangle$  does not depend on the choice of  $\phi$  (check!), and the equation above defines uniquely  $p$  a solution to detailed balance. It is easy to see that this solution is a probability (one has convergence as defined earlier

thanks to mass action semantics).  $\square$

One clearly sees two contributions here, the mass term  $z_0!/z!$ , and the flat term  $e^{-\langle K, \tilde{\phi} \rangle}$ .

*§thermodynamic rephrasing - free energy*

We can describe an equilibrium as the (free) energy assignment:

$$F(x) = \langle \epsilon, x \rangle + \log x! = \sum_{A \in S} \epsilon(A)x(A) + \sum_{A \in S} \log(x(A)!)$$

where  $\epsilon$  is such that  $K = C^t \epsilon$ .

Indeed:

$$-\log(p(z)/p(z_0)) = \log(z!) - \log(z_0!) + \langle K, \tilde{\phi} \rangle$$

and as  $K = C^t \epsilon$ :

$$\langle K, \tilde{\phi} \rangle = \langle C^t \epsilon, \tilde{\phi} \rangle = \langle \epsilon, C \tilde{\phi} \rangle = \langle \epsilon, z - z_0 \rangle = \langle \epsilon, z \rangle - \langle \epsilon, z_0 \rangle$$

so  $-\log(p(z)/p(z_0)) = F(z) - F(z_0)$ .  $\square$

NB: There is always an  $\epsilon$  such that  $K = C^t \epsilon$ , as  $\ker(C)^\perp =$



$Im(C^t)$ . There can be many, but then:

$$\begin{aligned}
 F_1(z) - F_2(z) &= \langle \epsilon_1 - \epsilon_2, z \rangle \\
 &= \langle \epsilon_1 - \epsilon_2, z_0 + C\tilde{\phi} \rangle \text{ for } \phi \text{ a path from } z \text{ to } z_0 \\
 &= \langle \epsilon_1 - \epsilon_2, z_0 \rangle \quad \text{because } \epsilon_1 - \epsilon_2 \in \ker(C^t) = Im(C)^\perp \\
 &= F_1(z_0) - F_2(z_0)
 \end{aligned}$$

which means that the energy difference is constant on a given component of the TG. Hence, restricted to any component, both variants define the same probability.

NB: One could also consider a vector-valued energy field  $f(x)(A) = \epsilon(A)x(A) + \log(x(A)!)$ , and then  $F(x) = |f(x)|_1$ .

We can evaluate the variation in free energy incurred by adding an  $A$ :

$$\begin{aligned}\mu_A &= \partial F / \partial x(A) \\ &= \partial \epsilon \cdot x / \partial x(A) + \partial \log x! / \partial x(A) \\ &= \epsilon_A + \log' x(A)! \\ &\sim \epsilon_A + \log x(A)\end{aligned}$$

using Stirling's  $\log n! = n \log n - n$ . This is called the chemical potential. Clearly, no matter how 'cheap' an  $A$  is (meaning how negative  $\epsilon_A$ ), eventually, the term  $\log x(A)$  will dominate and make the addition of a further  $A$  unlikely. This is the reason why numbers of tokens are kept in check (in thermodynamically correct reaction systems).

#### 4 Deconstructing entropy for Petri nets

We suppose from now on that  $|x| := \sum_A x(A)$  is an invariant  $n$  (ie the total number of tokens per component is constant; equivalently  $\mathbf{1} \in \mathbb{R}^S$  is an  $S$ -invariant; note that  $|x|$  is the  $L_1$  norm).

*§iii.i -*

What are the states that minimise  $E(x) := \sum_{A \in S} \epsilon(A)x(A)$ ?

Because  $|x| = n$ , the minimum is  $x = nA$  for  $A$  the species that has minimal  $\epsilon_A$ . This is an order term.

What are the states that minimise  $\sum_{A \in S} \log(x(A)!)$ ?

As  $|x| = n$  is fixed, to minimise  $\prod_{A \in S} x(A)!$  is the same as to maximise  $n! / \prod_{A \in S} x(A)!$  which is a multinomial coefficient (hence an integer), hence maximal for a uniform distribution of  $x(A)$ . This is a disorder term.

Since  $\pi(x) \propto e^{-F(x)}$ , those states  $x$  that minimise  $E(x)$  and maximise  $\Omega(x) := -\log x!$  will be favoured. Minimising the  $E$ -term is

easy, if  $A$  has the lowest  $\epsilon_A$ , then  $x$  should have as many as possible (order); maximising the  $\Omega$ -term is also easy,  $x$  should have a low  $x!$ , which means  $x$  should be as uniformly distributed among species as possible (as said above). The trouble comes from wanting to do both at once as the two goals are clearly contradictory!

*§iv -*

Consider the set of words  $S^n$  of length  $n$ , and write  $\pi$  for the (canonical) projection  $\pi$  from words to multisets.

For any  $x$ :

$$|\pi^{-1}(x)| = (\sum_A x(A))! / \prod_A x(A)! = n! / \prod_A x(A)!$$

The set of  $n! = (\sum_A x(A))!$  permutations over  $n$  acts on  $S^n$ , each induces an enumeration of the same underlying multiset  $x$  over  $n$ ; by the orbit-stabilizer lemma:

$$|\pi^{-1}(x)| \prod_A x(A)! = n!$$

note that  $w$ 's symmetry group is  $\prod_A x(A)!$ .

§v -

Define on  $S^n$ ,  $E(w) = \sum_{A \in w} \epsilon(A)$ . Clearly  $E(w)$  is constant on the class  $\pi^{-1}(\pi(w))$ .

Better, the equilibrium  $F$  is the image of  $E$  under the quotient induced by  $\pi$ , that is to say  $F(x) = E(w) + \log |\pi^{-1}(x)|$  up to an additive constant  $\log n!$ , for any  $w \in \pi^{-1}(x)$ .

In other words, we want to prove that the image under  $\pi$  of the equilibrium probability  $p_E$  on  $S^n$  is  $p_F$ , that is to say we want:

$$p_F(x) = \sum_{w \in \pi^{-1}(x)} p_E(w) = p_E(w) \cdot n! / \prod_A x(A)!$$

Taking a minus logarithm, we get:

$$F(x) = E(w) + \log x! - \log n!$$

so  $F(x) = E(w) - \Omega(x)$  up to an additive constant  $-\log n!$

What if  $n$  is not constant? We could take in this case:

$$E'(w) = \epsilon \cdot w - \log |w|! \tag{7}$$

to get a perfect match. Note that we are left with an ‘entropic’ term  $|w|!$  which does no longer depend on the repartition of species; is

that true to the intuition of getting rid of entropy? Note also that with  $E'$ , the energy variation of a concrete reaction  $w \rightarrow w'$  is  $\partial E + \log |w'|!/|w|!$ , so the constraint to be satisfied by the concrete transition system is now:

$$\log q(w', w)/q(w, w') = \langle \epsilon, \pi(w') - \pi(w) \rangle + \log |w'|!/|w|!$$

*§v.i - An aside on Multinomial coefficients*

Multinomial coefficients feature naturally in our problem. Using Stirling's approximation for the log of factorial, we can obtain nice asymptotic equivalents for multinomials.

A multinomial coefficient:

$$\binom{n}{n_1 \dots n_k} = \frac{n!}{n_1! \dots n_k!}$$

measures the number of partitions of  $n$  into  $k$  classes (some possibly empty),  $f : n \rightarrow k$ , such that the  $i$ th class has  $n_i$  elements, ie  $|f^{-1}(i)| = n_i$ .

It is also the coefficient of  $x_1^{n_1} \cdots x_k^{n_k}$  in  $(x_1 + \cdots + x_k)^n$ , hence the name.

Caveat: we are counting ordered partitions here, ie each class has a name, eg  $1, 2, 3 \mapsto 0, 1, 1 \neq 1, 2, 3 \mapsto 1, 0, 0$ , the former being associated to monomial  $xy^2$ , the latter to  $x^2y$ ;  $k = 2, n = 3$ , both coefficients are equal  $\binom{3}{12} = \binom{3}{21} = 3$ .

So:

$$k^n = \sum_{\{n_1, \dots, n_k \mid \sum n_i = n\}} \binom{n}{n_1 \cdots n_k}$$

$$\begin{aligned} \log(n! / \prod_{A \in S} x(A)!) &= \log n! - \sum_{A \in S} \log x(A)! \\ &\sim n(\log n - 1) - \sum_{A \in S} x(A)(\log x(A) - 1) \\ &= n \log n - \sum_{A \in S} x(A) \log x(A) \\ &= \sum_{A \in S} x(A) \log(n/x(A)) \\ &= n \sum_{A \in S} -(x(A)/n) \log(x(A)/n) \\ &= n \cdot S(x/|x|) \end{aligned}$$

where  $S$  is the usual entropy, and  $x(A)/|x|$  interpreted as the probability that an element of (some enumeration of)  $x$  is of type  $A$ .

So for large  $x$ s:

$$F(x) \sim E(x) - |x|S(x/|x|) = (\langle \epsilon \rangle - |S|)|x|$$

with  $\langle \epsilon \rangle = \sum_S \epsilon(A)x(A)/|x|$  the average energy of a random element; so if  $\langle \epsilon \rangle > \log |S|$  very roughly, then one should not produce too many particles.

*§vi - categorification of words, multisets and matches*

Construction of a concrete counterpart of  $N$  on  $S^n$  for which  $\pi$  is a strong stochastic bisimulation (an onto coalgebra morphism).

Let  $\mathbb{I}$  be the category of integers and injections.

Multisets over a finite set  $S$  are seen as objects in the product category  $\mathbb{I}^S$ . I.e a multiset is seen as a tuple of integers, and a morphism between such is a tuple of injections.

This supposes an order on  $S$  to describe the product. If one does not want an order, then an option is to describe multisets over  $S$  as functors from the discrete category  $S$  to  $\mathbb{I}$ , simply picking numbers



for species. Matches are natural transformations between such trivial functors:

$$\begin{array}{ccc} x(A) & \xrightarrow{\theta_A} & y(A) \\ I_{x(A)} \downarrow & & \downarrow I_{y(A)} \\ x(A) & \xrightarrow{\theta_A} & y(A) \end{array}$$

in this view a match is a map from  $S$  to finite injections, mapping an  $A$  to  $\theta_A$ , its components  $\theta_A$  entirely describe it. Everything is done pointwise.

Note that there are  $x!$  arrows from  $x$  to  $x$  - so maybe this should be the concrete TS?

The category  $\mathbb{E}_S$  of *enumerated multisets* over  $S$  can be described succinctly as the comma category of the inclusion function from  $\mathbb{I}$  to  $\mathbf{Set}_f$  (finite sets and maps) and the constant  $S$  functor from the one point category to  $\mathbf{Set}_f$  (picking up the base of our slice):

$$\mathbb{I} \rightarrow \mathbf{Set}_f \leftarrow 1$$

objects (ie words) are maps  $n \rightarrow S$ , arrows are injections that make

the triangle commute (expressing the preservation of types):

$$\begin{array}{ccc} n_1 & \xrightarrow{m} & n_2 \\ & \searrow w_1 & \swarrow w_2 \\ & S & \end{array}$$

If  $m$  is increasing,  $w_1$  is a *subword* of  $w_2$ . If  $m$  is a bijection, then  $w_1, w_2$  are permutation of one another, and conversely. This defines isomorphic words.

*[Could also use the cat of increasing maps  $\Delta$  as in simplicial complexes?]*

As mentioned before, we have the projection  $\pi : \mathbb{E}_S \rightarrow \mathbb{I}^S$  defined on objects as:

$$\pi(w)(A) = |\{w^{-1}(A)\}|$$

This is functorial from  $\mathbb{E}_S$  to  $\mathbb{I}^S$  - to see this we have to define  $\pi$  on matches.

Given  $m \in [w_1; w]$ ,  $A \in S$  we can restrict/localize/project  $m \in [w_1; w]$  to  $A$ , obtaining  $m_A \in [w_1(A); w(A)]$ , with  $w(A)$  the max subword of  $w$  made of  $As$ .

(This operation can be described as a pull-back - more later)

Then, the  $A^{th}$  component of  $\pi(m)$  is  $\pi(m)(A) = \hat{m}_A$ , where  $\hat{\cdot}$  chops off the slice basis  $S$ .

Concretely:

$$\begin{aligned}
 m &: & AAB & \xrightarrow[\substack{012 \\ 132}]{} & AABACB \\
 m_A &: & AA & \xrightarrow[\substack{01 \\ 12}]{} & AAA \\
 \pi(m)(A) &: & 2 & \xrightarrow[\substack{01 \\ 12}]{} & 3
 \end{aligned}$$

This “pointwise” action is functorial as  $\pi(I_w) = I_{\pi(w)}$  etc., it is faithful, and full (a bit like a covering space).

*§vi.i - base change*

The localization/max subword to/on  $A$  can be expressed as a pull-back under the trivial base change:

$$\begin{array}{ccc}
 n_A & \longrightarrow & n \\
 w(A)\downarrow & & \downarrow w \\
 \{A\} & \xrightarrow{j} & S
 \end{array}$$

So the definition of  $\pi(m)$  above can be seen as follows (front and back faces are pull-backs, side ones are injective arrows in the corresponding slice category):

$$\begin{array}{ccccc}
 & m_A & \longrightarrow & m & \\
 \pi(m)(A) \swarrow & \downarrow & & \searrow m & \downarrow \\
 n_A & \longrightarrow & n & & \\
 \downarrow & & \downarrow & & \downarrow \\
 & \{A\} & \longrightarrow & S & \\
 \swarrow 1 & & \searrow 1 & & \\
 \{A\} & \longrightarrow & S & & 
 \end{array}$$

NB: the notion of mass action, where one is counting injections (or subsets) already makes the matches of PNs concrete, and we see this better when things are couched in precise categorical terms.

*§vi.ii - lifting matches*

Given an order  $<$  on  $S$  (already assumed for the product representation of multisets), we can define a canonical enumeration, a right

inverse  $\pi^*$  to  $\pi$ , that is a map from multisets to words (collective to individual, fields to particles, etc):

$$x \mapsto w = \prod_{A \in \{S, <\}} x(A) \cdot A$$

where the product follows  $<$ ; eg:

$$\begin{array}{ccccc} AAB & \longrightarrow & 2A + B & \longrightarrow & AAB \\ \downarrow \begin{smallmatrix} 012 \\ 132 \end{smallmatrix} & & \downarrow \begin{smallmatrix} 01 & 0 \\ 12 & 0 \end{smallmatrix} & & \downarrow \begin{smallmatrix} 012 \\ 123 \end{smallmatrix} \\ AABACB & \longrightarrow & 3A + 2B + C & \longrightarrow & AAABBC \end{array}$$

we see  $\pi^*\pi$  is not the identity, its sorts objects.

*§vi.iii - lifting reactions*

For each reaction  $r = i(r) \rightarrow o(r)$  in  $R$ , with  $|i(r)| = |o(r)| = k \leq n$  (because of the invariant  $n$ ,  $k$  is the arity of  $r$ ), we thus obtain a concrete transition  $\hat{r}$  on  $S^n$  by canonically enumerating the multisets  $i(r)$  and  $o(r)$  using the order on  $S$ :

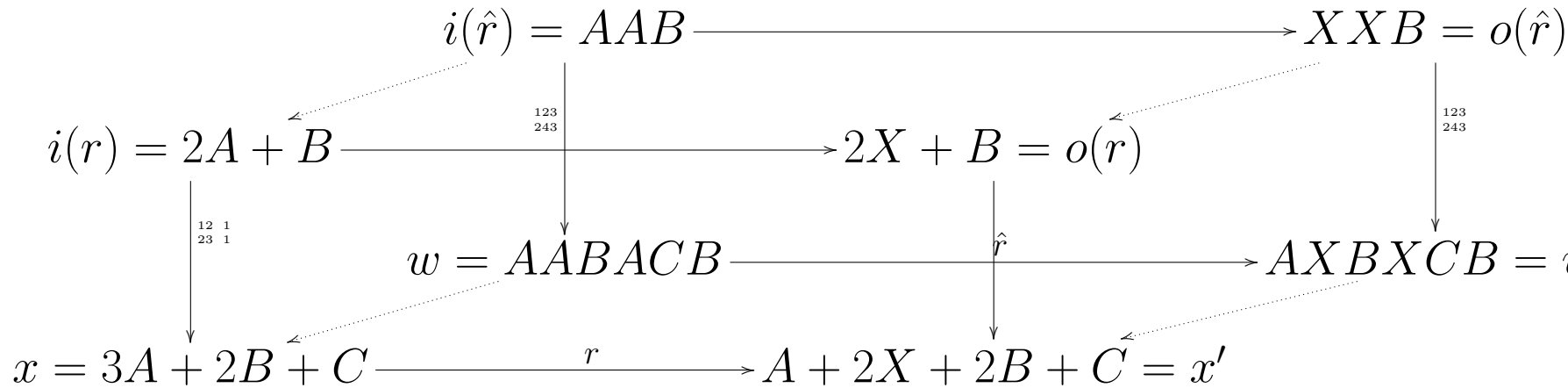
$$\hat{r} = \pi^*(i(r)) \rightarrow \pi^*(o(r))$$

This in turn defines a (mass action, ie event-based CTMC) rewrite system where subwords of length  $k$  are matched in words of length  $n$ , and substituted *in place* (by a subword of equal length  $k$  - still because  $n = |x|$  is invariant). We assign the same rate  $k(r)$  to  $\hat{r}$ .

[*Why in place? can we not append the rhs and delete the lhs? or something else? See below.*]

Write  $[w_1; w]$  for the set of matches for  $w_1$  in  $w$ , and given such a match  $m$ , write  $w[w_1 \setminus w_2 @ m]$  for the *in-place* substitution of  $w_2$  to  $w_1$ .

Here is an example of a concrete rewrite (back face):



Suppose  $x' = r \cdot x$ , one has:

$$\begin{aligned}
 q(w, \pi^{-1}(x')) &:= \sum_{w' \in \pi^{-1}(x')} q(w, w') && \text{by additivity of exit rates} \\
 &= k(r) \cdot |\{m \mid m \in [i(\hat{r}); w]\}| && \text{by simplicity of } N \\
 &= k(r) \cdot |\{\alpha \mid \alpha \in [i(r); x]\}| && \text{by f\&f of } \pi \\
 &= \sum_{m \in [i(\hat{r}); w]} q(w, w[i(\hat{r}) \setminus o(\hat{r}) @ m]) / \theta && \text{for some correction } \theta \\
 &= q(x, x')
 \end{aligned}$$

as any concrete transition from  $w$  -which by simplicity corresponds to a unique  $r$ - must preserve  $x'$ ; hence  $\pi$  is a (functional) stochastic bisimulation of CTMCs. Caveat:

$$k(r) \cdot |\{m \mid m \in [i(\hat{r}); w]\}| \neq \sum_{m \in [i(\hat{r}); w]} q(w, w[i(\hat{r}) \setminus o(\hat{r}) @ m])$$

since the map  $m \mapsto w[i(\hat{r}) \setminus o(\hat{r}) @ m]$  has no reason to be injective.

Eg above, we have  $w'$  invariant by preconjugation with  $12 \mapsto 21$  - in a way the micro-PN is *not simple* as the thickness of a concrete transition varies as a function of  $x$ . So the rhs is over-counting (in general), and one needs a correction for that (more later).

We ask: is the energy assignment  $E(w) = \sum_{A \in w} \epsilon(A) = \langle \epsilon, \pi(w) \rangle$  an equilibrium of the concrete counterpart of  $N$  as we have just defined?

*[it is well-known that bisim preserve equilibria; but here we are looking at lifting one, so the other direction; cf the Ehrenfest urn model of diffusion]*

*[we could also ask what is the energy function of the concrete system as defined, sans a priori]*

*§vii - an example*

Consider a simple sisma example with a single reversible reaction  $r = 3A \leftrightarrow A+2B$ ; since there is no non-trivial “loop” ( $R$ -invariant), this system has an equilibrium, and  $\epsilon_B - \epsilon_A = \kappa(r)$  (eg if both rate constants are set to 1,  $\epsilon_B = \epsilon_A$ ).

The energy assignment  $E(w)$  is consistent with the concrete TS constructed above if for any pair of related words  $w, w'$ , one has:

$$\log(q(w', w)/q(w, w')) = E(w') - E(w)$$



(NB: ratios of inverse jump rates depend only on  $\hat{r}$ ,  $r$  even, and not on the states  $w$ ,  $w'$ ).

Pick  $w$  with at least 3  $A$ s, and  $w'$  obtained by substituting two  $A$ s in  $w$  with  $B$ s, eg:

$$\begin{array}{ccc}
 AAA & \longrightarrow & ABB \\
 \downarrow & & \downarrow \\
 w = \dots AAA \dots & \xrightarrow{\hat{r}} & \dots ABB \dots = w' \\
 \downarrow \pi & & \downarrow \pi \\
 x & \xrightarrow{r} & x - 2A + 2B = x'
 \end{array}$$

In general, given  $w$ ,  $w'$ , we can uniquely determine  $r$  (by simplicity). We can also determine the *support* of the action of  $\hat{r}$ , meaning the subset of the image of the match  $m$  which is flipped/modified by the action  $\sigma$  (here - very easy to describe as length is not modified). So the thickness (or multiplicity) of a  $w, w'$  jump is going to be a product of two contributions:

-1) the nb of symmetries of the support of  $m$  in the target  $w$  that are preserved by the rule action  $\sigma$  (in our example this is 2, as both

As become  $B$ s);

- 2) the nb of matches of the fixed points in the remainder of  $w$  (in the example  $x(A) - 2$ )

So one has  $q(w, w') = k(r)(x(A) - 2)2!$ , with  $x(A)$  the number of  $A$ s in  $w$ , since the position of the non-substituted  $A$  does not change the result; similarly,  $q(w', w) = k(r^*)(x'(A) = x(A) - 2)2!$ ; hence  $\log q(w, w')/q(w, w') = \kappa(r)$ .

The entropy term  $\Omega$  is *explained away* by exhibiting a more concrete and microscopic version of the transition system. Can we do the same in general?

*§viii - general result - n invariant*

Write  $\sigma$  for the substitution associated to  $\hat{r}$  (only defined because we assume  $|x|$  constant), and suppose  $\sigma$  has no fixed points (no enzyme assumption), then we have:

$$m \cdot w = m' \cdot w \Leftrightarrow \exists \tau \in [w_1; w_1] : m\tau = m', \sigma\tau = \sigma$$

in other words, in this no enzyme case, the thickness of  $w \rightarrow w'$  is given by the number symmetries of  $w_1$  that are preserved by  $\sigma$  - this number is static, as it only depends on  $r$ .

In the enzymatic case it will depend on  $x$ , but not the ratio  $\kappa$  - see the example above - as by definition 'enzymes' figure on both sides.

One should also verify that this thickness is invariant under reaction reversal - so that the energy term indeed is  $E(w)$  (somehow, there is indirect evidence for this as the projection to  $F$  works?).

*§ix -*

It is unclear how this microscopic rendition of entropy can be extended from the assumption of an invariant number of tokens; one can no longer use the representation of events as substitutions  $\sigma$  - maybe by using insertions (as in the base category for simplicial complexes seen as presheaves); or by following the history of creation of a token (as in rCCS). Maybe we need to change the concrete rep-

resentation itself?

We have a fresh name problem.

Perhaps, try splits instead of squeezes (zigzags, quotients)?

*§x - why simple creation does not work*

Interpreting the ‘creation’ reaction  $r \Rightarrow A$  as appending  $A$  to a word is incompatible with our intended  $V$ . That is to say, with  $V(w) = \langle \epsilon, \pi(w) \rangle + \log |w|!$ , then we should have  $\log q(w', w)/q(w, w') = \epsilon(A) + \log |w'|$ , for any  $w, w'$  that one relate using  $r$ .

Consider the following concrete transition:

$$w = A^n B A^m \rightarrow A^n B A^{m+1} = w'$$

we compute the forward and backward rates:

$$q(w, w') = k(r) \times 1$$

$$q(w', w) = k(r^*) \times (m + 1) \text{ because erasing any of the } m + 1 \text{ As right of } B \text{ gives } w$$

so the log of the ratio is:

$$\begin{aligned}\log q(w', w)/q(w, w') &= \log k(r^*)/k(r) + \log(m + 1) \\ &\neq \partial V' = \epsilon(A) + \log(n + m + 2)\end{aligned}$$

unless  $n = 0$

[ $w'$  favours returning to  $w$ 's with a long tail of  $A$ 's, which flies in the face of the ratio being only dependent on the  $\partial V$ ]

*§xi - insertions uniformly at random*

One idea is to interpret the creation of  $A$  as *a uniform random insertion* of  $A$  in  $w$  in which case we get a new expression for the above ratio:

$$\begin{aligned}\log q(w', w)/q(w, w') &= \log k(r^*)/k(r) + \log(m + 1)/((m + 1)/(m + n + 2)) \\ &= \log k(r^*)/k(r) + \log |w'| \\ &= \partial V'\end{aligned}$$

The same computation work in general for any  $w, w'$  related by a creation. It remains to see if this works in general for any  $r$ , or

even before for any combined creation eg  $\rightarrow A + 2B$ , or concretely,  $+AAB$ .

What is the semantics of  $+AAB$ : to insert randomly each letter in turn.

(can we reduce to atomic creation?)

A general argument is that the set of steps from  $w$  to  $w'$ , that is a series of deletions  $-i(r)$  in  $w$ , followed by a series of insertions of  $o(r)$ , is isomorphic to that of steps for  $r^*$  leading from  $w'$  to  $w$  (this is the argument that underpins the proof above in the special case where  $r = +A$ ), (check!).

It follows that the non-constant part of  $\log q(w', w)/q(w, w')$  is (because of the uniform splitting of insertion rates):

$$\begin{aligned} \frac{\prod_{1 \leq i \leq |o(r)|} |w - i(r) + i|}{|w'|! / |w - i(r)|! / |w|! / |w - o(r)|!} &= \\ \frac{\prod_{1 \leq i \leq |o(r^*)|} |w' - i(r^*) + i|}{|w'|! / |w|!} &= \\ |w'|! / \cdot |w|! & \end{aligned}$$