Jordan Algebra AChems:
Exploiting Mathematical Richness for Open Ended Design

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Abstract

We identify some desired mathematical properties of bonds in an Artificial Chemistry (AChem) that promote complexity and open-ended behaviour (i.e. an AChem not designed to display particular behaviours). We identify the underlying structures created by different properties of mathematical products. We use these to exploit existing algebra to generate a potentially open-ended subsymbolic AChem (ssAChem). We give examples of how our approach leads to interesting behaviour, focused on the structure of composite particles within our system.

A Low Level Approach to Artificial Chemistries

Most Artificial Chemistries (AChems) seek to produce a system capable of displaying specific behaviours associated with abiogenesis, the transition from inorganic to organic (living) materials (Hutton, 2002; Lucht, 2012; Suzuki et al., 2003). Those systems succeed in generating their particular behaviours because that is what they are designed to do. Another approach is to consider that we are seeking open-ended behaviour in our systems. In order to design for open-ended behaviour we need to approach the problem in an open-ended way.

We need to design a system that is rich and complex, with properties that allow us to define all the reactions of our AChem implicitly. We can then start looking for, and finding, behaviours that are emergent from the design, rather than engineered explicitly. We need a set of building blocks and connectors that do not limit the structure we design. Think of this as the difference between a prefabricated house and a brick house. A prefab has pieces that are specifically designed to fit together and form a house, and have a limited capability to do anything else. A brick house is just the bricks and the mortar that joins them. The bricks are not limited to building a certain house, or even a house of a particular size. With enough bricks and mortar the possibilities are endless. Likewise in an open-ended AChem the only limit should be the material and the amount of energy in the system.

We need to consider desirable properties of the interactions of our particles, rather than of the whole system, while ensuring that we do not over- or under-constrain the AChem. Here we do this by taking a mathematical approach, and taking advantage of existing mathematical theory and structures. This allows us to discuss not just the properties and behaviours of the particles, but also the different links and linking structures between them. We can then use established mathematics that has many emergent properties with interesting forms of interactions. We can also expand our view to talk about the effects of these properties on the system as a whole.

Terminology

Dittrich et al. (2001) define an AChem as a triple (S, R, A), where S is the set of possible molecules, R the set of rules for binding molecules, and A an algorithm describing the dynamics of the environment.

Rather than talking of 'molecules', we refer to the members of S as *particles*; these are either atomic particles (*atoms*) or composite particles (*composites*). Rather than talking of 'bonds', we say that the rules R say how particles can be joined together with *links*; links can be broken to decompose composite particles. We use this terminology to help prevent confusion between the properties of real chemical molecules and our AChem particles, and to prevent the abuse of chemistry terminology.

Faulconbridge et al. (2010) introduce the concept of *subsymbolic* AChems (ssAChem), with an example based on RBN-world. Such AChems have an implicit rule set where the properties used by the rules emerge from the internal structure of the particles. RBN-world was further developed in (Faulconbridge et al., 2010; Faulconbridge, 2011).

Here we demonstrate how the algebraic properties of the chosen rule set can be exploited to help obtain rich structures, and demonstrate this with an ssAChem based on a Jordan algebra of Hermitian matrices.

Mathematical Properties and Structure of Composite Particles

Our ssAChem rules have two parts: a set of mathematical products (or mathematical operations) for forming links and composites, and a set of probabilities used to determine probability of a reaction. In this section we discuss the properties of the mathematical product.

In mathematics there are two properties of a product on a set that are easily defined, and that can be indicative of many further properties of an algebra. These are associativity and commutativity.

$$\text{Associativity:} \quad (a \circ b) \circ c = a \circ (b \circ c) \quad (1)$$
$$\text{Commutativity:} \quad a \circ b = b \circ a \quad (2)$$

When we have a binary product, thereby linking two particles, combinations of these properties lead to four distinct structures, Table 1.

For an associative, commutative binary product we can change the order of evaluation and the ordering within any evaluation. No matter how we link a given set of particles, we get the same result. The structure is a bag. For an associative, non-commutative binary product we can change the order of evaluation such that there is no ordering on the products, but we cannot change the ordering within the product; the structure is a string.

Associativity is an assumed property of most algebras. Non-associative algebras, while rare, normally appear in an applied setting. They have been used in connection with genetics (Reed, 1997) and physics (McCrimmon, 1978) as well as a broad range of applications to mathematical theory (Gonzalez and Martinez, 2003). One of their main attractions is that with their enforced evaluation order they can embody a loose form of time, or at least an ordering of interactions.

For a non-associative, commutative product we can re-order particles in a product, but we have an enforced order of products. The structure is a binary tree, with unordered child nodes. For a non-associative, non-commutative product, we have an enforced order of products and ordering of particles within the products. The structure is a graph, with complicated directionality restrictions requiring labelling on both edges and nodes; these are not simple structures and do not conform to any of the normally used graph subtypes.

Let us consider these four structures in terms of an AChem. A bag has no internal structure, and limits us to a set of composite particles with the cardinality of the power set of the component particles. In real chemistry there are *isomers*: molecules with different inherent properties despite containing the same atoms in different arrangements (Muller, 1994). Isomers add complexity and increase the size of the combinatorial space. An AChem with a bag structure has no equivalent of isomers, so we do not want to base ours on an associative commutative product.

Associativity	Commutativity	Structure
Yes	Yes	Bag
Yes	No	String
No	Yes	Tree
No	No	Graph

Table 1: Summary of structure provided by different mathematical properties

Strings are structures that have received a lot of attention in the computing community, but they are rather simple mathematical objects that lack room for expansion. They have very simple combinatorial power of

$$C_{n-1} = \frac{(2n-1)!}{n!(n-1)!} \quad (3)$$

Strings support analogues of isomers, but there are not many of them. There is also no ordering of operations, so how they are formed does not affect the result. So we reject associative non-commutative products.

The tree structure given by the non-associative commutative product not only has more room for expansion to larger trees, it also has an implicit ordering. Because we cannot change the order of operations we get a variety of structures, and a system in which structure is as important as the building blocks themselves. This gives us a system with greater intrinsic flexibility.

The graph structure of a non-associative non-commutative product provides yet more structure, but makes it hard for the product to have any regularity to exploit as it allows so many possible structures. It is not necessary that we work with a structure this complex so we stick to trees.

Larger products

We can look beyond binary products to products that take more arguments, combining multiple particles with a common link.

This does not affect the structure of the system if we have an associative non-commutative product: since it is associative this changes nothing and we still have a string. However in the case of the non-associative commutative product as we expand from a binary product to a larger product we move from a binary tree to a general tree.

There are a larger number of possible trees with $n \geq 4$ leaves than strings with $n \geq 4$ elements. For $n = 3$ we have $s_3 = 6$ and $t_3 = 4$, where s_n is the number of strings with n elements and t_n is the number of trees with n leaves. For $n = 4$ we have $s_4 = 24$ and $t_4 = 31$ using products of any size, see Figure 1. We can show that from this point onward there is a larger number of possible trees than strings.

The number of possible strings increases with n such that $s_{n+1} = s_n(n+1)$. For trees we have a faster growth. We can

(a) $1\times$

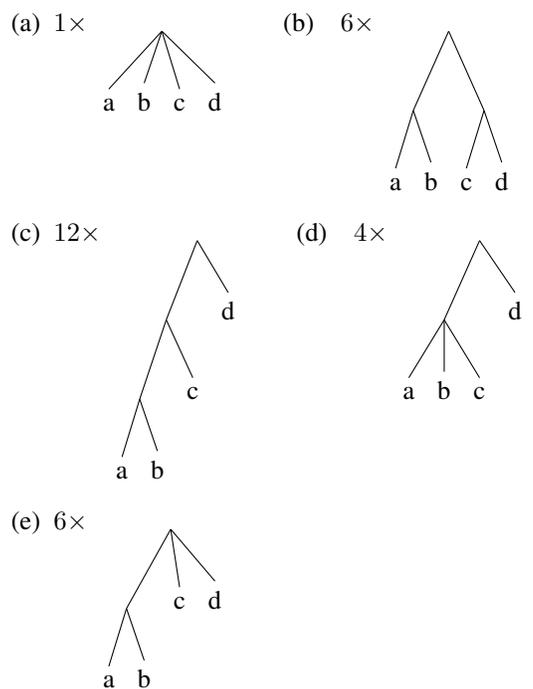(b) $6\times$

(c) $12\times$

(d) $4\times$

(e) $6\times$

Figure 1: Tree structures with four leaves with multipliers indicating the number of relevant rearrangements of leaves, giving an indication of all possible trees with four leaves with in this system.

show that if we link the extra element to the result of each of the graphs with n nodes with a binary link then the new element can be swapped with any of the other elements to give at least $t_{n+1} \geq t_n(n+1)$. We also always have more graphs as this does not include the graph of the $(n+1)$-product (see Figure 2) making t_{n+1} strictly greater than $t_n(n+1)$. Thus as we have more trees at $n = 4$ and a faster growth in the trees than in the strings, for $n \geq 4$ we always have more possible trees than strings.

In terms of an AChem, these properties show that we have a more interesting selection of possibilities in a non-associative system than otherwise, and these possibilities are controlled by the order in which reactions occur. Hence we focus on non-associative commutative products for our ssAChem design.

Jordan Algebras

Having established that these mathematical properties are desirable, we need to find a system in which we have these properties. Mathematics as a field has already found and studied systems with such properties, in the case of non-associative commutative systems we have Jordan Algebras (McCrimmon, 2006).

Jordan Algebras were originally conceived to find a solution to describing observables in quantum mechanics, but

(a)

subtree size i n_{i+1}

(b)

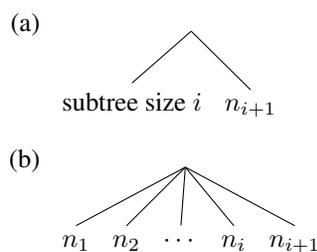n_1 n_2 $\cdots$ n_i n_{i+1}

Figure 2: Trees showing greater growth than strings

were later discarded for that purpose because none of the Jordan Algebras were able to solve the problem. They have two important properties which define them:

$$\text{Jordan identity:} \quad (x \bullet y) \bullet x^{\bullet 2} = x \bullet (y \bullet x^{\bullet 2}) \quad (4)$$

where $x^{\bullet n} = x \bullet x \bullet \cdots \bullet x \quad (n \text{ times})$

$$\text{Power associative:} \quad x^{\bullet m} x^{\bullet n} = x^{\bullet (m+n)} \quad \forall m, n \geq 0 \tag{5}$$

Power associativity tells us what happens when we work with just one kind of particle.

There are several Jordan Algebras (McCrimmon, 2006). Here we take the most accessible Jordan Algebra that exists over the Hermitian matrices (a matrix is Hermitian if it equals its Hermitian conjugate, see Equation 14).

With this Jordan Algebra we start with a binary product formed of familiar matrix multiplication and addition to define the Jordan product:

$$X \bullet Y := \tfrac{1}{2}(XY + YX) \tag{6}$$

As one can see $X \bullet Y = Y \bullet X$. It is also non-associative:

$$(X \bullet Y) \bullet Z = \tfrac{1}{2}(XY + YX) \bullet Z \tag{7}$$
$$= \tfrac{1}{4}(XYZ + YXZ + ZXY + ZYX) \tag{8}$$
$$\neq \tfrac{1}{4}(XYZ + XZY + YZX + ZYX) \tag{9}$$
$$= \tfrac{1}{2}X \bullet (YZ + ZY) \tag{10}$$
$$= X \bullet (Y \bullet Z) \tag{11}$$

One of the advantages of a non-associative algebra is the ability to expand from the binary product and the binary tree it creates to a general product and its general tree. We can expand the binary product linearly to give the Jordan triple product:

$$\{X, Y, Z\} = (X \bullet (Y \bullet Z) + (X \bullet Y) \bullet Z - (X \bullet Z) \bullet Y)$$
$$= \tfrac{1}{2}(XYZ + ZYX) \tag{12}$$

We can further extend this to an arbitrary length n product, called an n-tad in Jordan theory (McCrimmon, 2006):

$$\{X_1, X_2, \cdots, X_n\} = \tfrac{1}{2}(X_1 X_2 \cdots X_n + X_n \cdots X_2 X_1) \tag{13}$$

Using the n-tad notation, $(X \bullet Y) = \{X, Y\}$.

Commutativity of this product means that we can fully reverse the order of the elements in the product, but not freely rearrange the order completely. So there is a large number of possible n-tad products for a particular set of n objects, increasing our combinatorial power and the ability of our system to exploit some properties of composite particles. Thus Jordan Algebras equip us with products that are open-ended, and are applicable to the open set of Hermitian matrices.

Mathematical Objects

Other AChems have used 'matrices' as the basis of their set S. In particular, the binary string chemistry (Banzhaf, 1993), dubbed the matrix-multiplication chemistry by Dittrich et al. (2001), makes use of matrix multiplication. However, it does not treat its particles as mathematical objects; rather, it folds binary strings into a matrix in order to give a simpler definition of a function over the binary strings. This is common for the use of 'matrices' in systems that use 'matrix' to mean a two dimensional storage array rather than the mathematical object that we use here.

All of the previous discussion in this paper has been building towards creating a system that uses mathematical objects for both the particles *and* links of our system. This is the beauty of a mathematical product: it is in some ways an object with properties in its own right.

Additionally, the matrices themselves are rich in emergent properties that might be exploited by our system.

Hermitian Matrices and Subsymbolic Artificial Chemistries

The atoms in the Jordan ssAChem used here are 3×3 Hermitian matrices.

Hermitian matrices use the Hermitian conjugate of a complex matrix:

$$\begin{pmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{pmatrix}^{\dagger} = \begin{pmatrix} \bar{a_{11}} & \bar{a_{21}} & \bar{a_{31}} \\ \bar{a_{12}} & \bar{a_{22}} & \bar{a_{32}} \\ \bar{a_{13}} & \bar{a_{23}} & \bar{a_{33}} \end{pmatrix} \quad (14)$$

The elements a_{ij} are complex numbers, and $\bar{a}$ is the complex conjugate of a. A matrix M is Hermitian if $M = M^{\dagger}$. Hermitian matrices are closed under the Jordan product (McCrimmon, 2006).

Hermitian matrices provide a rich variety of properties such that we can use them as prime material for creating a subsymbolic AChem (ssAChem) where emergent properties of the matrices dictate the linking capabilities/probabilities of a particle, and the algebra gives the structure of the composite particles.

In this work we use the eigenstates of the Hermitian Matrices, chosen for their dimensionality and spatiality, and because they are a well studied mathematical object. A fully worked example of linking, probabilities and strengths generated using Hermitian matrices is given in the Appendix.

Subsymbolic Link

We make use of the eigenstate of the matrix to define linking probabilities. For a matrix M, consider

$$Mv = \mu v \quad (15)$$

The solution vectors v_i are the eigenvectors; the corresponding scalars μ_i are the eigenvalues. Here we choose these unit eigenvectors and the corresponding normalised eigenvalues λ_i as our emergent properties of interest to define our linking probabilities:

$$\lambda_i = \mu_i / \sum \mu_j \quad (16)$$

We normalise the eigenvalues to ensure sensible linking probabilities of larger composites.

The probability of two particles A and B linking, based on a given pair of eigenvalues and eigenvectors, is defined to be:

$$p_{A_i B_j} = \mathcal{N}(\lambda_{A_i} - \lambda_{B_j}) \left(1 - \tfrac{1}{2}((v_{A_i} \cdot v_{B_j}) + 1)\right) \quad (17)$$

This has two parts. The first term $\mathcal{N}(\lambda_{A_i} - \lambda_{B_j})$ is the probability density of the normal distribution ($\mu = 0, \sigma = 1$) at the point given by the difference in the normalised eigenvalues. This means the probability of linking is larger for more similar normalised eigenvalues. The normal distribution is not the only option; we simply need a symmetric distribution centred on zero, and the normal distribution is a well-known such one.

The second term $(1 - \tfrac{1}{2}((v_{A_i} \cdot v_{B_j}) + 1))$ uses the dot product between the corresponding unit eigenvectors. The dot product between two unit vectors is the cosine of the angle between them. The overall term has a value between 0 and 1, and is 0 if the vectors are perfectly aligned and 1 if the vectors are anti-aligned.

The probability of two particles linking, p_{AB}, is defined as the maximum probability of all the possible pairs:

$$p_{AB} = \max\{p_{A_i B_j} \; \forall i, j\} \quad (18)$$

The other property we define from the eigenstate is the strength of the link (probability that the link does not decompose). This is based solely on the difference in the normalised eigenvalues:

$$l_{A \bullet B} = \mathcal{N}(\lambda_{A_i} - \lambda_{B_j}) \quad (19)$$

Both these properties are based on the binary product. We define the linking probability of a triple link to be:

$$p_{ACB} = \min\{p_{AC}, p_{CB}\} \quad (20)$$

and we use the same set of eigenvalues to generate the links strength as the minimum of the strengths for each of the pairs $[\lambda_{A_p}, \lambda_{C_q}]$ and $[\lambda_{C_r}, \lambda_{B_s}]$:

$$l_{\{ACB\}} = \min\left\{\mathcal{N}(\lambda_{A_p} - \lambda_{C_q}), \mathcal{N}(\lambda_{C_r} - \lambda_{B_s})\right\} \quad (21)$$

This can be extended to the n-tad case in a similar fashion.

Composite Particles Probability

In our system the links have properties of their own. Equation 18 is the probability of the link forming given the presence of its components and that we choose that many reactants.

We need a further two probabilities to work out the probability of the resulting composite of the link existing, f_A. We need a probability of a particle existing, e_A:

$$e_A = \begin{cases} 1 & \text{if } A \text{ is an atom} \\ f_A & \text{if } A \text{ is a composite} \end{cases} \quad (22)$$

And we need a probability that each particle takes part in the reaction. All reactions that form a link require us to select at least two components. We define the probability of selecting further components for the reaction as 0.1 for each component. This choice discourages our system from constantly forming large links and quickly becoming one large composite.

$$r_{\{A_1, \cdots, A_n\}} = 0.1^{n-2} \quad (23)$$

So together the probability of a composite forming in terms of its last link is:

$$f_X = f_{\{A_1, \cdots, A_n\}} = p_X r_X \prod_{i=1}^{n} e_{A_i} \quad (24)$$

Composite Particles Strength

Link strength in our system is truly a property of the link rather than the composite. The composite particle contains a series of links all with different properties; each link has the link strength given in Equation 19. The overall composite strength is given by the probability of each of the links not decomposing, and is the product of all the link strengths in the system. The result is that larger links are stronger than a series of smaller links as there is less chance for the composite to break down. This is given by:

$$s_X = \prod_{Y \subset X} l_Y \quad (25)$$

where l_Y is the link forming Y a sub-particle of X.

Structure

The Jordan Algebra underlying this system means that the structure of the composite is as important as the particles that make it up. Through this we can see that not only does the structure add to the properties of the composite, but also we can find behaviour in the structure independent of the particles. By this we find the analogue of an *isomer* from real chemistry.
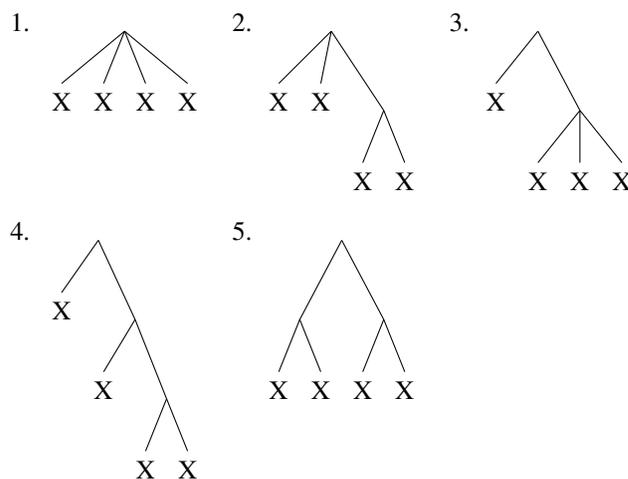

Figure 3: The set of structural isomers of four identical atoms

Isomer	Probability	Strength	Maximum reaction size	No. links
I1	0.0020	0.3989	4	1
I2	0.0040	0.1592	3	2
I3	0.0040	0.1592	3	2
I4	0.0079	0.0635	2	3
I5	0.0079	0.0635	2	3

Table 2: Particle probability and particle strength for the isomers of the identity atom (isomers 1 to 5 with X=I).

An Example of Emergent Richness

Throughout we have talked about the richness of the Jordan Algebra basis for this system and how it allows us to create a system in which we can have meaningful isomers. We can see this most clearly when we consider the homomers (isomers containing only one kind of particle) generated by the identity matrix, I, which is also an identity under the Jordan product (and hence all these composites are also represented by I).

There are five possible structural isomers using just four atoms I (Figure 3). Each of these has a probability of forming and a strength (Table 2).

From these results we can see that in the simplest of circumstances (when we are looking only at the structure of the isomer), structures with larger links are harder to form but once created are also harder to destroy. Thus we have emergently created a system that has stronger and weaker structures depending on the way the composite particle forms.

These multiple link isomers can form links with particles of different matrices, which have different eigenvalues. We give a second example of a base particle for which the five

Isomer	Probability	Strength	Maximum reaction size	No. links
M1	0.0019	0.3774	4	1
M2	0.0037	0.1476	3	2
M3	0.0037	0.1496	3	2
M4	0.0073	0.0585	2	3
M5	0.0070	0.0557	2	3

Table 3: Particle probability and particle strength for the isomers of the M atom (isomers 1 to 5 with X=M).

resultant homomers behave differently. Consider the matrix M:

$$M = \begin{pmatrix} 1 & i & 0 \\ -i & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \qquad (26)$$

The isomers formed from M all result in the same final matrix, as is true of all homomers due to the power associativity law (Equation 5). Since all the component matrices have the same eigenvectors, we never have a product occurring with the same eigenvalue position, as they are perfectly aligned and so the linking probability is zero (Equation 17). This increases the strength and probability of larger links as all pairs in the link can form across the strongest link because there is no case in which both possible link positions are occupied.

These results show that isomers are all unique: the structure is not defined by size or number of links (otherwise isomers M2, M3 or M4, M5 would be identical). This also shows that the structure has a strong effect on the system. The link properties are changing because we are no longer working with the identity matrix, and the composites are different from M. Thus when we link with the larger composite particles, eg $((M \bullet M) \bullet M)$, we are in fact linking with a different set of eigenvalues (if not necessarily a different set of eigenvectors as discussed previously). This still gives us a pattern of decreased probability of creation and increased strength for a smaller number of larger links.

We can also see that this behaviour does not indicate a universal pattern of higher probability causing lower strength regardless of other properties. Isomer M4 has a higher probability than isomer M5 but also has a higher strength. We can also see that these do not stretch across different homomers as I isomer I1 is more probable than M isomer M1 and is also stronger. This means that it is not the relationship between probability and strength that causes this behaviour, it is a relative effect caused by differently structured homomers of the same size.

While the probabilities given for the existence of composites existing here are small and tending towards zero for larger composites we must remember that this system is intended to operate over a very large number of interactions.

Thus while the probability of any particular composite existing is small particularly for larger composites the chance of generating a (large) composite is relatively high given the number of possible (large) composites.

Other Possible Behaviours

This is not the only interesting behaviour we might find which results directly from non-associativity and a mathematical focus.

Firstly we may consider looking at the isomers of our system in order to understand the more general behaviours of isomers. We can look at the probabilities of large molecules forming and their ability to act as information storage and transfer. We can be certain from the design of the system that the formation and replication of large composite particles is possible. However we cannot be sure of how stable or regular these large composites would be. If they are not stable then they cannot act as an information storage and transfer mechanism as the data would have too high a probability of corrupting. If they are not sufficiently regular then the information stored in them cannot be read in any useful manner.

The concepts of catalysis and substitution are fairly well established behaviors looked for in AChems (Hutton, 2003; Faulconbridge et al., 2010; Hickinbotham et al., 2010; Suzuki et al., 2003). Many other systems implement these concepts in addition to their basic reaction mechanism. We could create additional capability in our system to enable catalysis and substitution, but it is not necessary. This is because we have a probabilistic system. If we have two particles, A and B, that have a low probability of linking then we can use a composite particle C to generate a larger particle $((A \bullet C) \bullet B)$ (Figure 4). When we decompose in the correct manner this can leave us with a composite $(A \bullet B)$ whose total probability of forming is much higher than the original probability of A, B linking directly. It is even possible that this would allow objects with perfectly aligned eigenvectors, which would normally have a linking probability of 0, to connect and have a strong resultant link.

Another well-established desirable behaviour is replication. We have not eliminated self-replication. In this system it would look like a composite forming and then it being used much like C in Figure 4 to help the formation of an identical composite. Interesting instances of this would be cases in which the copy has a higher probability of existing than the original. This would mean that the composite encourages the creation of copies of itself.

Considering the analogy to real chemistry, we will at some point want to consider adding a temperature analogue to our system. This should modify the probability of linking in the system. In this case it could modify either the eigenvalues or the eigenvectors of the matrix. There are very few ways to do this that do not effect both of these, so as well as changing the probability of linking we would be caus-
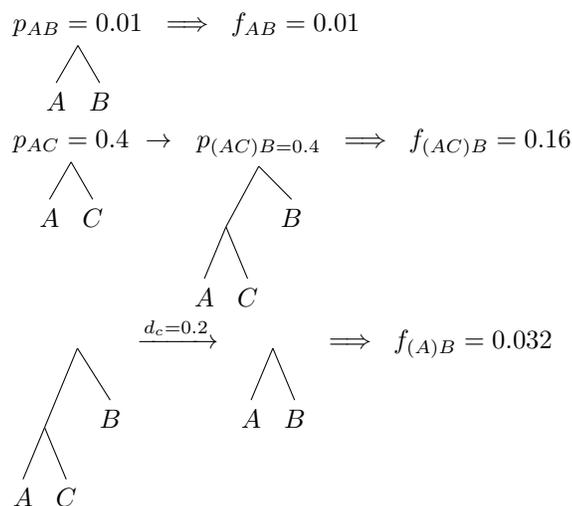
$$p_{AB} = 0.01 \implies f_{AB} = 0.01$$

$$p_{AC} = 0.4 \rightarrow p_{(AC)B=0.4} \implies f_{(AC)B} = 0.16$$

$$\xrightarrow{d_c=0.2} \implies f_{(A)B} = 0.032$$

Figure 4: A general example of what the concept of catalysis would look like in our system where d_C is the probability of C decomposing in the correct manner.

ing the composite to "rotate". The structure of the matrices provide for a direct connection between an analogue of thermal energy and its effects on the energetic states (such as rotational or kinetic energy) of our composite particles. In addition, in our system variation of temperature should lead to increasing and decreasing probabilities, similar to the effects in ensembles in real chemistry as described by statistical thermodynamics.

Summary and Conclusions

Creating an AChem using a mathematical basis such that links and ordering exists gives us a chance to exploit the open set of Hermitian matrices and their already well-studied emergent properties. It also provides us with structure that exists and is capable of displaying emergent behaviours that cannot be predicted purely from the mathematical roots of the system.

We have shown that even within the power associativity provided by the Jordan Algebra the fact that the underlying system is non-associative allows for these strong structural influences to become more prevalent and vary the system. We have also discussed that this may not remain the case when expanded to general isomers but will remain true in homomers.

We have demonstrated that we can find interesting important behaviors in this sort of ssAChem that were in no way designed into our system. This suggests that these systems have much greater potential in that they are not being limited by the intentions and goals of their creators. In terms of our starting metaphor, we are starting to create bricks and mortar, rather than a prefabricated AChem.

Appendix: worked example

Linking Hermitian Matrices

Consider the three Hermitian matrices:

$$X = \begin{pmatrix} 1 & -i & i \\ i & 0 & 0 \\ -i & 0 & 0 \end{pmatrix} \quad Y = \begin{pmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{pmatrix}$$

$$Z = \begin{pmatrix} -1 & i & 0 \\ -i & -1 & 0 \\ 0 & 0 & 0 \end{pmatrix} \tag{27}$$

These have the following eigenvector matrices and eigenvalues:

$$X : v_X = \begin{pmatrix} 0.58i & 0 & 0.82 \\ 0.58 & 0.71 & -0.41 \\ -0.58 & 0.71 & 0.41 \end{pmatrix} \lambda_X = \begin{pmatrix} -1 & 0 & 2 \end{pmatrix} \tag{28}$$

$$Y : v_Y = \begin{pmatrix} 0.41 & 0.71 & 0.58 \\ 0.41 & -0.71 & 0.58 \\ -0.82 & 0 & 0.58 \end{pmatrix} \lambda_Y = \begin{pmatrix} 0 & 0 & 3 \end{pmatrix} \tag{29}$$

$$Z : v_Z = \begin{pmatrix} -0.71i & -0.71i & 0 \\ 0.71 & 0.71 & 0 \\ 0 & 0 & 1 \end{pmatrix} \lambda_Z = \begin{pmatrix} -2 & 0 & 0 \end{pmatrix} \tag{30}$$

We can form three links over these matrices, using the relevant products:

1. $(X \bullet Y) = \begin{pmatrix} 1 & \frac{1}{2} - \frac{1}{2}i & \frac{1}{2} + \frac{1}{2}i \\ \frac{1}{2} + \frac{1}{2}i & 0 & 1i \\ \frac{1}{2} - \frac{1}{2}i & -1i & 0 \end{pmatrix}$

2. $\{X, Y, Z\} = \begin{pmatrix} -1 & 1i & -\frac{1}{2} - \frac{1}{2}i \\ -1i & -1 & \frac{1}{2} - \frac{1}{2}i \\ -\frac{1}{2} + \frac{1}{2}i & \frac{1}{2} + \frac{1}{2}i & 0 \end{pmatrix}$

3. $((X \bullet Y) \bullet Z) = \begin{pmatrix} -\frac{3}{2} & -\frac{1}{2} + 1i & -\frac{3}{4} - \frac{1}{4}i \\ -\frac{1}{2} - 1i & -\frac{1}{2} & \frac{1}{4} - \frac{3}{4}i \\ -\frac{3}{4} + \frac{1}{4}i & \frac{1}{4} + \frac{3}{4}i & 0 \end{pmatrix}$

Link Properties

For each of these links we can calculate the probability of the link, L, forming, p_L, and the strength of the link, l_L. In order to calculate the probability of L we need to calculate the probability using each possible choice of eigenvalues. Taking link 1 we have the probabilities as given in Table 4 the maximum of which occurs using the second eigenvalues

p	X_1	X_2	X_3	Z_1	Z_2	Z_3
Y_1	0.035	0.257	0.041	0.086	0.142	0.362
Y_2	0.170	0.299	0.019	0.182	0.299	0.200
Y_3	0.027	0.242	0.121	0.118	0.072	0.051

Table 4: Probability of linking with Y for X and Z for each eigenvalue

p	Z_1	Z_2	Z_3
$(X \bullet Y)_1$	0.0270	0.1210	0.0354
$(X \bullet Y)_2$	0.0782	0.2700	0.0997
$(X \bullet Y)_3$	0.1638	0.0175	0.0135

Table 5: Probability of $(X \bullet Y)$ linking with Z for each eigenvalue

of X and Y, this gives us a probability $p_{XY} = 0.2992$ and a strength of $l_{XY} = 0.3989$. These along with the strength and probability of the other two links are summarized in Table 6.

For link 2 we take the minimum of the probabilities p_{XY} and p_{YZ}. The probabilities for p_{YZ} are also given in Table 4 and the maximum occurs with Y's first eigenvalue and Z's third eigenvalue. This gives $p_{YZ} = 0.3623$ which has a strength of $l_{YZ} = 0.3989$. We then have that the overall $p_{XYZ} = 0.2992$ and it has strength $l_{XYZ} = 0.3989$.

For link 3 we need to work out a third set of probabilities between $(X \bullet Y)$ and Z, these will be based on the eigenstate of $X \bullet Y$ (Table 5):

$$(X \bullet Y) : V_{(X \bullet Y)} = \begin{pmatrix} 0 & -0.5 - 0.5i & 0.5 + 0.5i \\ -0.71i & 0.5i & 0.5i \\ 0.71 & 0.5 & 0.5 \end{pmatrix}$$

$$\lambda_{(X \bullet Y)} = \begin{pmatrix} -1 & 0 & 2 \end{pmatrix} \tag{31}$$

This means the largest probability comes from using the second eigenvalues of each component and so $p_{(XY)Z} = 0.2700$ which makes the strength $l_{(XY)Z} = 0.3989$.

Composite Properties

We next consider the f and s values for the composite resulting from each link. The first link has only atoms and is binary so $f_{XY} = p_{XY}$ and since there is only one link the strengths are also the same: $s_{XY} = l_{XY}$. Similarly $s_{XYZ} = l_{XYZ}$ as there is only one link but $f_{XYZ} \neq p_{XYZ}$ as the size of the link reduces the probability to $f_{XYZ} = 0.1 p_{XYZ} = 0.0299$.

Finally we have the probability of the third link: $f_{(XY)Z} = p_{XY} p_{(XY)Z} = 0.0808$. The base components are atoms and the links are all binary so it is simply the product of the probabilities of both links. The strength is the product of the strengths of each link: $s_{(XY)Z} = l_{XY} l_{(XY)Z} = 0.1591$.

Link	Probability	Strength	Composite Probability	Composite Strength
1	0.2992	0.3989	0.2992	0.3989
2	0.2992	0.3989	0.0299	0.3989
3	0.2700	0.3989	0.0808	0.1591

Table 6: Summary of links probabilities and strengths

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