# COUNTING CHEMICAL REACTION NETWORKS WITH NAUTY

MURAD BANAJI

Abstract. It is useful to have lists of unlabelled (i.e., nonisomorphic) chemical reaction networks (CRNs), with or without various restrictions such as reversibility. One may, for example, be interested in exploring how often certain dynamical behaviours occur in small CRNs, or wish to search for examples to illustrate some aspect of the theory. In such cases, it is often natural to examine all nonisomorphic CRNs in the class of interest. Inspired by the related project of Deckard *et al* [1], this document outlines some interesting classes of CRNs, and the methodology involved in listing all CRNs in these classes. The accompanying data (i.e., lists of nonisomorphic CRNs in the various classes) is at `https://reaction-networks.net/networks/`.

## 1. Introduction

When discussing the combinatorial structure of a chemical reaction network (CRN), the basic objects are the chemical species, the complexes and the reactions. Suppose that the species of a CRN are $\mathrm{X}_1, \ldots, \mathrm{X}_k$. A *complex* is a formal linear combination of species of the form $a_1\mathrm{X}_1 + a_2\mathrm{X}_2 + \cdots + a_k\mathrm{X}_k$ where each $a_i$ is a nonnegative integer, the *stoichiometry* of $\mathrm{X}_i$ in the complex. A complex $a_1\mathrm{X}_1 + a_2\mathrm{X}_2 + \cdots + a_k\mathrm{X}_k$ such that $\sum_i a_i \leq 2$ is termed an *at most bimolecular* complex, or a **2-complex** for short. The *zero complex* $0\mathrm{X}_1 + \cdots + 0\mathrm{X}_k$ is denoted 0 (note that 0 is a 2-complex). An ireversible reaction is an ordered pair of complexes, the *source complex* (or left hand side of the reaction) and the *target complex* (or right hand side of the reaction). Thus any chemical reaction on the set of species $\{\mathrm{X}_i\}$ takes the form

$$\sum_i a_i\mathrm{X}_i \to \sum_i b_i\mathrm{X}_i$$

Such a reaction is *at most bimolecular* if its source and target complexes are 2-complexes. From here on, at most bimolecular CRNs will be termed **2-CRNs**, and only 2-CRNs are treated; the modifications required if larger stoichiometries are allowed are fairly straightforward.

By basic principles of choice with repetition, there are

$$n_C(k) := \binom{k+2}{2}$$

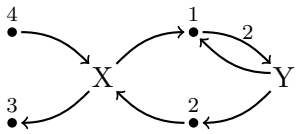
2-complexes on $k$ species, including the zero complex.

1.1. **The complex graph, and basic restrictions: no loops or parallel edges.** A CRN $\mathcal{R}$ is just a set of chemical species and a set of reactions, and is then naturally identified with its *complex graph*, the digraph whose vertices are the complexes of the network and whose arcs are its (irreversible) reactions. Two common conventions about CRNs adopted here are

(1) The source and target complexes of a reaction are distinct: the complex graph has no loops.
(2) Two distinct reactions cannot have the same source and target complexes: the complex graph has no parallel arcs (antiparallel arcs are of course allowed, corresponding to reversible reactions).

The first of these conventions is quite natural, while the second is more arbitrary: with certain choices of kinetics allowing the same reaction to figure more than once can enlarge the set of allowed models of a CRN, while for others (most importantly, mass action) it cannot.

1.2. **Petri net graphs and isomorphism.** For the purposes of discussing isomorphism, the most useful representation of a CRN is via its *Petri net (PN) graph* [2], an edge-weighted bipartite digraph (equivalently, since edge-weights are positive integers, a bipartite multidigraph). The PN graph of a CRN $\mathcal{R}$, denoted $PN(\mathcal{R})$, has two vertex sets $V_S$ (species vertices) and $V_R$ (reaction vertices). Given $\mathrm{X}_i \in V_S$ and $R_j \in V_R$, there exists an arc $\mathrm{X}_i R_j$ (resp., $R_j \mathrm{X}_i$) with weight $w$ if and only if the species $\mathrm{X}_i$ occurs with stoichiometry $w$ on the left (resp., right) of the reaction $R_j$. For example, the PN graph of $\mathrm{X} + \mathrm{Y} \to 2\mathrm{Y}$, $\mathrm{Y} \to \mathrm{X} \rightleftharpoons 0$ takes the form:




Arc-weights of 1 have been omitted and reaction vertices have been given numerical labels. CRNs $\mathcal{R}_1$ and $\mathcal{R}_2$ are isomorphic if $PN(\mathcal{R}_1)$ and $PN(\mathcal{R}_2)$ are isomorphic in the following natural sense: there exists a relabelling of the vertices of $PN(\mathcal{R}_1)$ which preserves the bipartition and gives $PN(\mathcal{R}_2)$. This accords with the intuition that two CRNs are fundamentally "the same" if some renaming of species and reactions in one gives us the other. Isomorphism is of course an equivalence relation on the set of CRNs and we refer to an equivalence class of isomorphic CRNs as an *unlabelled CRN*.

1.3. **ODE models.** In order to describe some interesting classes of CRNs we need brief mention of differential equation models of CRNs.

A real vector $x = (x_1, \ldots, x_k)^t$ is nonnegative (resp., positive) if $x_i \geq 0$ (resp., $x_i > 0$) for each $i$. The set of nonnegative (resp., positive) vectors in $\mathbb{R}^k$ is denoted $\mathbb{R}^k_{\geq 0}$ (resp., $\mathbb{R}^k_{\gg 0}$). Subsets of $\mathbb{R}^k_{\gg 0}$

are referred to as positive. $x \gg 0$ means $x_i > 0$ for each $i$; $x \geq 0$ means $x_i \geq 0$ for each $i$; $x > 0$ means $x \geq 0$ and $x \neq 0$.

Consider a CRN $\mathcal{R}$ involving $k$ chemical species $X_1, \ldots, X_k$ with corresponding concentration vector $x = (x_1, \ldots, x_k)^t$ and $m$ irreversible reactions. Choosing some orderings on the species and reactions one can define nonnegative $n \times m$ matrices $L$ and $R$ as follows: $L_{ij}$ (resp., $R_{ij}$) is the stoichiometry of species $X_i$ in the source complex (resp., target complex) of reaction $j$. The *irreversible stoichiometric matrix* of $\mathcal{R}$ is $\Gamma = R - L$. The $j$th column of $\Gamma$ is termed the *reaction vector* for the $j$th reaction.

If the reactions of $\mathcal{R}$ proceed with rates $v_1(x), v_2(x), \ldots, v_m(x)$, then the evolution of the species concentrations is then governed by the ODE:

$$\dot{x} = \Gamma v(x). \tag{1}$$

where $v(x) = (v_1(x), v_2(x), \ldots, v_m(x))^t$ is the *rate function* of $\mathcal{R}$. The allowed choices of $v(x)$ depend on various modelling choices; but many reasonable choices imply that $v(x) \gg 0$ for any $x \gg 0$. In this case we say that $\mathcal{R}$ has *positive kinetics*.

## 2. Counting unlabelled CRNs with NAUTY [3]: the basic classes

While NAUTY does not allow direct operation on edge-labelled digraphs or multidigraphs, these can be represented as layered digraphs. I.e. individual vertices become sets of vertices, additional vertex colouring is introduced, and edges with different labels become edges between vertices of different colours as described in the section *Isomorphism of edge-coloured graphs* of the NAUTY documentation at `http://users.cecs.anu.edu.au/~bdm/nauty/nug26.pdf`. Via this process, a 2-CRN with $k$ species and $l$ reactions can be represented as an ordinary digraph on $2(k+l)$ vertices with edges labelled 1 or 2 now corresponding to arcs between different sets of vertices in the digraph. In this form, a CRN is in fact a digraph with *four* vertex colours, two corresponding to different layers of species vertices, and two corresponding to different layers of reaction vertices. (Indeed, an at most trimolecular CRN can be represented as a digraph on $2(k + l)$ vertices, but if larger total stoichiometry is allowed, then additional vertices need to be introduced.) NAUTY can be used to canonically label digraphs while respecting the partition of the vertices, and so we can get a canonical representative of a given CRN, by first converting it to a digraph, applying NAUTY's canonical labelling, and then converting back to a CRN.

### 2.1. Counting irreversible 2-CRNs.

All unlabelled 2-CRNs with $k$ species and $l$ reactions can be generated as follows:

(1) irreversible reactions are *ordered* pairs of distinct complexes: consequently there are a total of

$$n_R(k) := n_C(k)(n_C(k)-1)$$

distinct irreversible reactions involving the $n_C$ 2-complexes;

(2) all possible sets of $l$ distinct reactions are generated and stored as edge-labelled digraphs, represented (in `digraph6` format) as two-layer vertex-coloured digraphs as described in the NAUTY user guide at `http://users.cecs.anu.edu.au/~bdm/nauty/nug26.pdf`. There are

$$N_{k,l} := \binom{n_R(k)}{l} = \binom{\binom{k+2}{2}\left(\binom{k+2}{2}-1\right)}{l}$$

of these CRNs; for fixed $k$ and $l$ small compared to $\binom{k+2}{2}\left(\binom{k+2}{2}-1\right)$, $N_{k,l}$ grows quite rapidly. For example:

$$N_{4,1} = 210, \quad N_{4,2} = 21945, \quad N_{4,3} = 1.52 \times 10^6, \quad N_{4,4} = 7.87 \times 10^7, \quad \dots$$

(3) the NAUTY program `shortg` is used to canonically label and remove isomorphs from this list of CRNs, respecting the species-reaction bipartition. We are left with $\overline{N_{k,l}}$ unlabelled CRNs. For example:

$$\overline{N_{4,1}} = 22, \quad \overline{N_{4,2}} = 1171, \quad \overline{N_{4,3}} = 67257, \quad \overline{N_{4,4}} = 3.33 \times 10^6, \quad \dots$$

**Remark 2.1** (Maximally dense CRNs)**.** *A 2-CRN with $k$ species can have no more than $n_R(k) = \binom{k+2}{2}\left(\binom{k+2}{2}-1\right)$ reactions. The unique 2-CRN with $k$ species and $n_R(k)$ reactions can be thought of as a maximally "dense" CRN with $k$ species, which contains all other $k$-species 2-CRNs as subnetworks obtained by removing some reactions.*

**Remark 2.2** (Automorphisms of CRNs)**.** *Each labelled CRN on $k$ species lies in an isomorphism class consisting of upto $k!$ CRNs (corresponding to each possible permutation of the species). The actual size of the isomorphism class is less than $k!$ if and only if the CRN has nontrivial symmetries. For example the CRN $A \to B \to C \to A$ has nontrivial symmetry: its automorphism group is isomorphic to $\mathbb{Z}_3$ and consequently its isomorphism class has size $6/3 = 2$. Looking at the numbers, the great majority of CRNs with more than a few species and reations have no nontrivial symmetries. For example, $N_{4,4}/\overline{N_{4,4}} \simeq 23.65$, namely, the average orbit size of the 4 species, 4-reaction CRNs is close to $4!$.*

2.2. **Counting reversible 2-CRNs.** All *reversible* unlabelled 2-CRNs with $k$ species and $l$ reversible reactions can be generated similarly to the irreversible case. A 2-CRN with $k$ species and $l$ reversible reactions is of course a CRN with $k$ species and $2l$ irreversible reactions. However the reversible 2-CRNs are best enumerated directly as follows.

(1) Reversible reactions are *unordered* pairs of distinct complexes: consequently there are a total of $n_R^r(k) := \binom{n_C(k)}{2}$ of these;
(2) all possible sets of $l$ distinct reversible reactions are generated and stored as edge-labelled digraphs, represented (in `digraph6` format) as two-layer vertex-coloured digraphs. There are
$$N_{k,l}^r := \binom{n_R^r(k)}{l} = \binom{\binom{\binom{k+2}{2}}{2}}{l}$$
of these CRNs;
(3) the NAUTY program `shortg` is used to canonically label and remove isomorphs from this list of CRNs, respecting the species-reaction bipartition. We are left with $\overline{N_{k,l}^r}$ unlabelled CRNs. By comparison with the numbers above for irreversible reactions, for example:
$$\overline{N_{4,1}^r} = 13, \quad \overline{N_{4,2}^r} = 325, \quad \overline{N_{4,3}^r} = 8713, \quad \overline{N_{4,4}^r} = 205948, \quad \dots$$

2.3. **Using invariants.** The size of the enumeration problem grows rapidly with the number of species and reactions. For example, there are $N_{4,5} = 3{,}244{,}032{,}792$ labelled CRNs with four species and five reactions which fall into $\overline{N_{4,5}} = 135{,}622{,}844$ isomorphism classes. It becomes natural – and indeed necessary – to divide up the raw unlabelled CRNs using invariants which are easily computed before attempting to remove isomorphs. Thus one might, for example, divide up the raw CRNs according to how many edges with edge-label 2 they have, before using `shortg` to remove isomorphs from each list, and finally merging the lists. Some of the larger sets of CRNs at `https://reaction-networks.net/networks/` were enumerated in a multi-stage process in this way. However, even with the use of invariants, handling the $N_{5,5} = 106{,}337{,}815{,}584$ labelled CRNs with five species and five reactions on a desktop becomes challenging! Just storing these CRNs in (uncompressed) `digraph6` format would take about 6 terabytes of space. On the other hand parsing the data several times leads to a large increase in terms of simulation time. Dealing with these issues is work in progress.

2.4. **Enumeration by inheritance.** In the light of the explosion in problem size, an alternative to enumerating labelled CRNs and then separating these into isomorphism classes is to build larger CRNs from smaller ones. For example, given representatives from each isomorphism class of CRNs with $k$ species and $l$ reactions, we may hope to build the unlabelled CRNs with $k$ species and $l+1$ reactions as follows: we take each CRN with $k$ species and $l$ reactions, and add to it every possible reaction on $k$ species which does not already occur in it; we then remove isomorphs from this list of CRNs with $k$ species and $l+1$ reactions. This certainly gives a complete list of nonisomorphic CRNs with $k$ species and $l+1$ reactions, since the removal of any reaction from a CRN with $k$ species and $l+1$ reactions leaves a valid CRN with $k$ species and $l$ reactions.

Note, however, that we cannot interchange species and reactions in this approach: there are valid CRNs with $k+1$ species and $l$ reactions, which do not contain any valid induced subnetworks with $k$ species and $l$ reactions. As an example consider the CRN

$$A + B \to A,\ B \to A + B.$$

Removal of $A$ leaves $B \to 0$, $B \to B$, while removal of $B$ leaves $A \to A$, $0 \to A$, neither of which is a valid CRN (recall that in our definition of a CRN, source and target complexes of each reaction are distinct). Thus this CRN has no induced subCRNs involving 1 species and 2 reactions, and so cannot be built by adding species into a CRN involving 1 species and 2 reactions.

## 3. Counting interesting subclasses of CRNs

The raw CRNs enumerated as described in the previous section may be interesting from a purely combinatorial point of view, but we may wish to exclude some of them for various reasons. Below is a (far from exhaustive) list of some interesting subclasses of CRNs with some comments on their enumeration.

### 3.1. **Genuine CRNs.**

The definition of a CRN does not exclude the possibility that some species participate in no reactions. However, when analysing CRNs with $k$ species and $l$ reactions one may want to exclude ones with species which figure in no reactions (corresponding to isolated species vertices in the PN graph). CRNs which do not have such trivial species are termed *genuine* (for want of a better word).

**Remark 3.1** (Maximum number of species in a genuine CRN)**.** *Since an at most bimolecular reaction involves a maximum of* 4 *species, clearly a genuine 2-CRN with* $l$ *reactions can have and more than* $4l$ *species.*

**Remark 3.2** (Counting genuine CRNs given the numbers for all CRNs)**.** *The number* $\overline{N^G_{k,l}}$ *of unlabelled genuine CRNs with* $k$ *species and* $l$ *reactions is easily seen to satisfy*

$$\overline{N^G_{k,l}} = \overline{N_{k,l}} - \overline{N_{k-1,l}}\,.$$

*This follows because the* $k$*-species,* $l$*-reaction CRNs which are* not *genuine are exactly those obtained from* $(k-1)$*-species* $l$*-reaction CRNs via addition of a redundant species.*

### 3.2. **Indecomposable CRNs.**

More generally, one may wish to exclude CRNs with disconnected PN graphs (namely CRNs whose species can be divided into two nonempty non-interacting subsets). We refer to CRNs with disconnected PN graphs as *decomposable*, while CRNs with connected PN graphs are *indecomposable*. If we are interested in searching for new dynamical behaviours which arise in larger CRNs, then exluding decomposable CRNs is natural, as their dynamics decouples into that of the smaller CRNs of which they are composed.

**Remark 3.3** (Indecomposable CRNs are genuine)**.** *The indecomposable CRNs are clearly a subset of the genuine CRNs.*

3.3. **Dynamically nontrivial CRNs.** We might also wish to exclude CRNs which are in some way uninteresting from a dynamical point of view. Consider a CRN $\mathcal{R}$ consisting of $k$ species and $l$ irreversible reactions with $k \times l$ stoichiometric matrix $\Gamma$. $\mathcal{R}$ is referred to as *dynamically trivial* if there exists a linear scalar function which increases along all positive orbits for any positive kinetics (see Section 1.3), and *dynamically nontrivial* otherwise. Equivalently, $\mathcal{R}$ is dynamically trivial if there exists a vector $q > 0$ in $\operatorname{im}\Gamma^{\mathrm{t}}$. To see the equivalence, note that given $p$ s.t. $\Gamma^{\mathrm{t}}p = q > 0$, for any kinetics such that $x \gg 0 \Rightarrow v(x) \gg 0$, we have

$$\frac{\mathrm{d}}{\mathrm{d}t}p^{\mathrm{t}}x = p^{\mathrm{t}}\dot{x} = q^{\mathrm{t}}v(x) > 0$$

and thus $p^{\mathrm{t}}x$ increases along orbits at every point in $\mathbb{R}^k_{\gg 0}$.

By standard arguments, a dynamically trivial CRN $\mathcal{R}$ can have no limit sets intersecting $\mathbb{R}^k_{\gg 0}$. If we are primarily interested in CRNs which potentially admit positive equilibria, periodic orbits, chaos, etc., then we would wish immediately to exclude the dynamically trivial CRNs.

**Remark 3.4.** *Note that to state that a CRN is dynamically nontrivial only implies the nonexistence of an increasing linear functional; we do not claim that for a dynamically nontrivial CRN there* must *exist some positive limit points of the flow for arbitrary positive kinetics.*

**Remark 3.5** (Testing whether a given CRN is dynamically trivial)**.** *This is a linear programming feasibility problem, which can be solved, for example, with the help of the linear programming package* GLPK *(http://www.gnu.org/software/glpk/glpk.html ).*

3.4. **Weakly reversible CRNs.** Another class of CRNs which may be of interest are the *weakly reversible* CRNs. A CRN is weakly reversible if every connected component (CC) of its complex graph is a strongly connected component (SCC). Let $\Gamma$ be the stoichiometric matrix of a CRN $\mathcal{R}$ consisting of irreversible reactions.

**Remark 3.6** (Weakly reversible CRNs are dynamically nontrivial)**.** *As is well known and easily proved, if $\mathcal{R}$ is weakly reversible, then* $\ker\Gamma$ *includes a positive vector. Consequently,* $\operatorname{im}\Gamma^t$ *includes no vector* $> 0$ *(Theorem 3' in* [4]*, for example) and the claim follows.*

**Remark 3.7** (Reversible CRNs are weakly reversible)**.** *This is immediate from the definitions.*

**Remark 3.8** (Testing for weak reversibility)**.** *The test for whether a CRN $\mathcal{R}$ is weakly reversible is a standard graph theoretic test on the complex graph of $\mathcal{R}$. We can, for example, take each CC and check if it is an SCC using Tarjan's algorithm.*

3.5. **Fully open CRNs.** An important and highly studied subclass of CRNs are the "fully open CRNs". One possible interpretation of "fully open" would be to class a CRN with stoichiometric matrix $\Gamma$ as fully open if $\operatorname{rank}\Gamma$ (namely, the dimension of the stoichiometric subspace, $\operatorname{im}\Gamma$) is equal to the total number of species. Equivalently, the system has no linear first integrals. However, for some purposes it is useful to adopt a stricter notion (see, for example, [5]): here, a CRN involving species $\mathrm{X}_1, \ldots, \mathrm{X}_k$ is defined to be *fully open* if and only if it includes all the reactions $0 \rightleftharpoons \mathrm{X}_i$ $(i = 1, \ldots, k)$. Reactions not of the form $0 \to \mathrm{X}_i$ or $\mathrm{X}_i \to 0$ are termed *non-flow reactions.*

**Remark 3.9** (Fully open CRNs are genuine and dynamically nontrivial)**.** *Clearly a fully open CRN is genuine. It is also easily seen that a fully open CRN is dynamically nontrivial.*

One way of enumerating fully open CRNs with $k$ reactions and $l$ non-flow reactions is to consider all CRNs with $k$ reactions and $l$ reactions and remove any which include a reaction of the form $0 \to \mathrm{X}_i$ or $\mathrm{X}_i \to 0$. Noting that two fully open CRNs are isomorphic if and only if they are isomorphic after removal from both of the flow reactions $0 \rightleftharpoons \mathrm{X}_i$, these are now precisely the fully open CRNs with all the reactions $0 \rightleftharpoons \mathrm{X}_i$ removed.

Alternatively fully open CRNs may be enumerated directly. This proceeds in a similar fashion to enumerating general CRNs. We describe the process for the general case; the special case of fully open, reversible, CRNs is easily obtained via minor modifications. All unlabelled, fully open CRNs with $k$ species and $l$ non-flow reactions can be generated as follows:

(1) As already noted there are a total of $n_C(k)(n_C(k)-1)$ distinct irreversible reactions involving all 2-complexes; from these we exclude reactions of the form $0 \to \mathrm{X}_i$ and $\mathrm{X}_i \to 0$ leaving $n_{R,o}(k) := n_C(k)(n_C(k)-1) - 2k$ distinct non-flow reactions;
(2) all possible sets of $l$ distinct non-flow reactions are enumerated. There are
$$N^o_{k,l} := \binom{n_{R,o}(k)}{l} = \binom{\binom{k+2}{2}\left(\binom{k+2}{2}-1\right) - 2k}{l}$$
of these CRNs;
(3) the NAUTY program `shortg` is used to canonically label and remove isomorphs from this list of CRNs, respecting the species-reaction bipartition. These CRNs are precisely the set of all fully open CRNs with the reactions $0 \rightleftharpoons \mathrm{X}_i$ removed.

Although the numbers $N^o_{k,l}$ grow almost as fast as the numbers $N_{k,l}$, note that a fully open CRN with $k$ species and $l$ non-flow reactions is actually a CRN with $k$ species and $l + 2k$ reactions, and a much greater proportion of fully open CRNs with $k$ species and $l$ non-flow reactions are likely to be dynamically interesting than the corresponding proportion for CRNs with $k$ species and $l$ reactions.

**Remark 3.10.** *The fully open CRNs stored at* `https://reaction-networks.net/networks/` *have the reactions* $0 \to \mathrm{X}_i$ *and* $\mathrm{X}_i \to 0$ *removed. Thus to reconstruct the fully open CRNs from the stored networks, these need to be added.*

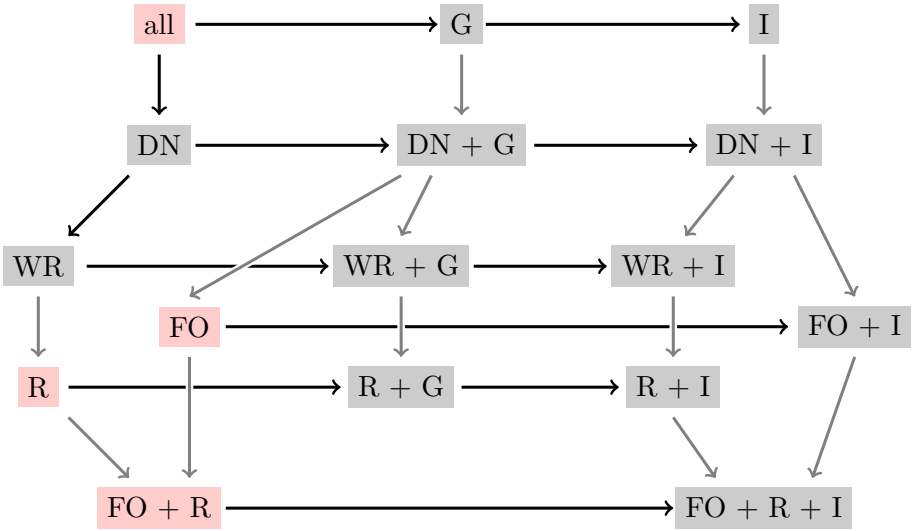
Fully open, reversible, CRNs can be enumerated similarly:

(1) From the $\binom{n_C(k)}{2}$ distinct reversible reactions we exclude the reactions $0 \rightleftharpoons \mathrm{X}_i$ leaving $n^r_{R,o}(k) := \binom{n_C(k)}{2} - k$ distinct reversible non-flow reactions;
(2) all possible sets of $l$ distinct reversible non-flow reactions are enumerated. There are $\binom{n^r_{R,o}(k)}{l}$ of these CRNs. These are precisely the set of all fully open reversible CRNs with the reactions $0 \rightleftharpoons \mathrm{X}_i$ removed.
(3) `shortg` is used to canonically label and remove isomorphs from this list of CRNs, respecting the species-reaction bipartition.

**Remark 3.11.** *The fully open, reversible, CRNs stored at* `https://reaction-networks.net/networks/` *have the reactions* $0 \rightleftharpoons \mathrm{X}_i$ *removed. Thus to reconstruct the fully open, reversible CRNs from the stored networks, these need to be added.*

## 4. Relationships among classes of CRNs discussed

Inclusions amongst the various classes of 2-CRNs discussed here are illustrated in the diagram below. $A \to B$ means $A \supseteq B$, and in fact all the inclusions are strict. The following acronyms are used: DN = dynamically nontrivial, WR = weakly reversible, FO = fully open, R = reversible, G = genuine, I = indecomposable.



The sets "all", "fully open", "reversible" and "fully open, reversible" (highlighted in red) are directly enumerated as described above. The remaining sets are enumerated by taking some parent set (connected to the set via a bold arrow) and checking for additional properties. For example, the dynamically nontrivial CRNs are obtained from the set of all CRNs by testing each CRN for the property of being dynamically nontrivial; the weakly reversible CRNs are obtained from the set of all dynamically nontrivial CRNs by testing each for the property of weak reversibility; the set "DN + G" is obtained from "DN" by testing each CRN for the property that it has no isolated species. And so forth.

## References

[1] A. Deckard, F. Bergmann, and S. Herbert. Enumeration and online library of mass-action reaction networks. `http://arXiv.org/abs/0901.3067`, 2009.

[2] D. Angeli, P. De Leenheer, and E. D. Sontag. A Petri net approach to the study of persistence in chemical reaction networks. *Math. Biosci.*, 210:598–618, 2007.

[3] B. D. McKay and A. Piperno. Practical graph isomorphism II. *J. Symbolic Computation*, 60:94–112, 2013.

[4] A. Ben-Israel. Notes on linear inequalities, 1: The intersection of the nonnegative orthant with complementary orthogonal subspaces. *J. Math. Anal. Appl.*, 9:303–314, 1964.

[5] M. Banaji and C. Pantea. The inheritance of nondegenerate multistationarity in chemical reaction networks. preprint at `https://arxiv.org/abs/1608.08400`.