The stoichBondGraph Module: From Stoichiometry to Bond Graph

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Contents

Note: this is the stoichBondGraph.ipynb notebook. The PDF version "The stoichBondGraph module: From Stoichiometry to Bond Graph" is available here.

1 Introduction

The bond graph approach (Oster et al., 1971, 1973; Gawthrop and Crampin, 2014; Gawthrop et al., 2015; Gawthrop and Crampin, 2016, 2017) to modelling biomolecular systems of interest to systems biologists developed independently from the stoichiometric approach (Palsson, 2006, 2011, 2015).

However, the conceptual point of intersection of the two approaches is the fact that the stoichiometric matrix is the modulus of the conceptual multiport transformer linking reactions to species. This means that the two approaches are complementary and each can build on the strengths of the other.

This tutorial illustrates how a stoichiometric system description can be used to automatically create the corresponding bond graph. However, more compex systems such as the ecoli core model (Orth et al., 2010) can also be translated in the same way.

1.1 Import some python code

The bond graph analysis uses a number of Python modules:

```
In [1]: ## Some useful imports
        import BondGraphTools as bgt
        import numpy as np

        ## Stoichiometry to BG
        import stoichBondGraph as stbg
```

2 Create a stoichiometric representation

In this context a stoichimetric representation is a python dictionary with the following fields

- name (string): the name of the bg to be created
- N (numpy integer array): the stoichiometric matrix
- species (list of strings): the names of the species
- reaction (list of strings): the names of the reaction

Optionally, the forward and reverse stoichometric matrices Nf and Nr can be included instead of N

Note that there is one species per row, and one reaction per column, of N

A file name.py is written containing the function model() which returns the bg in bgt form

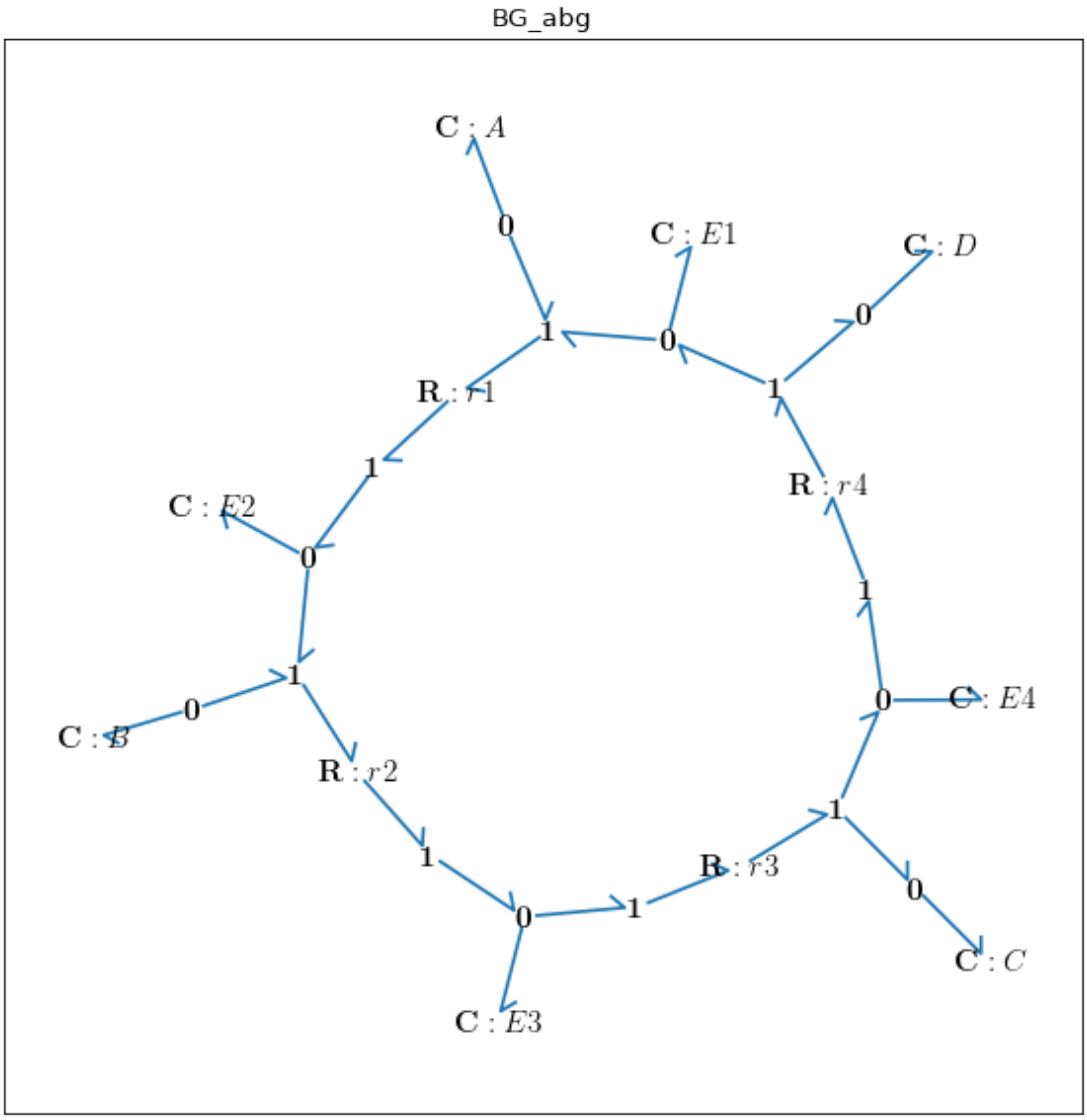
2.1 Example

This example corresponds to ABCD_abg.svg in Tutorial svgBondGraph.

In [2]:
```
## Stoichiometric matrix N
N = np.array(
    [
     [-1, 0, 0, 0],
     [ 0,-1, 0, 0],
     [ 0, 0, 1, 0],
     [ 0, 0, 0, 1],
     [-1, 0, 0, 1],
     [ 1,-1, 0, 0],
     [ 0, 1,-1, 0],
     [ 0, 0, 1,-1]
    ]
)

## Species and reactions
species = ['A', 'B', 'C', 'D', 'E1', 'E2', 'E3', 'E4']
reaction = ['r1', 'r2', 'r3', 'r4']

## Pack into a dict with name 'ABCDE_abg'
s = {
    'name':'BG_abg',
    'N':N,
    'species':species,
    'reaction':reaction
    }

## Convert to a bondgraph
stbg.model(s)

## And import
import BG_abg
```

2.2 Draw the BG

In [4]:
```
## Draw the BG
bgt.draw(BG_abg.model())
```



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